

Modified spectral parameter power series representations for solutions of Sturm-Liouville equations and their applications

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Abstract

Spectral parameter power series (SPPS) representations for solutions of Sturm-Liouville equations proved to be an efficient practical tool for solving corresponding spectral and scattering problems. They are based on a computation of recursive integrals, sometimes called formal powers. In this paper new relations between the formal powers are presented which considerably improve and extend the application of the SPPS method. For example, originally the SPPS method at a first step required to construct a nonvanishing (in general, a complex-valued) particular solution corresponding to the zero-value of the spectral parameter. The obtained relations remove this limitation. Additionally, equations with “nasty” Sturm-Liouville coefficients $1/p$ or r can be solved by the SPPS method.

We develop the SPPS representations for solutions of Sturm-Liouville equations of the form

$$(p(x)u')' + q(x)u = \sum_{k=1}^N \lambda^k R_k[u], \quad x \in (a, b)$$

where $R_k[u] := r_k(x)u + s_k(x)u'$, $k = 1, \dots, N$, the complex-valued functions p , q , r_k , s_k are continuous on the finite segment $[a, b]$.

Several numerical examples illustrate the efficiency of the method and its wide applicability.

1 Introduction

Solutions of sufficiently regular linear second order Sturm-Liouville equations considered as functions of a spectral parameter are entire functions which in particular means that they admit a normally convergent Taylor series representation in terms of the spectral parameter in the whole complex plane. The coefficients of the series are functions of the independent variable. For example, in the simplest case of the equation $y''(x) = \lambda y(x)$ two linearly independent solutions (satisfying in the origin the initial conditions $(1, 0)$, $(0, 1)$) can be chosen in the form $y_1(x) = \cosh \sqrt{\lambda}x$ and $y_2(x) = (\sinh \sqrt{\lambda}x) / \sqrt{\lambda}$. The Taylor coefficients in their power series in terms of the spectral parameter λ with the center $\lambda = 0$ are powers of the independent variable divided by corresponding factorials $x^{2n}/(2n)!$ and $x^{2n+1}/(2n+1)!$ respectively.

In [16] a simple way for calculating the Taylor coefficients for spectral parameter power series (SPPS) defining solutions of the Sturm-Liouville equation $(pu')' + qu = \lambda u$ was proposed, based on the theory of complex pseudoanalytic functions. In [18] (see also [17]) that result was extended onto equations of the form

$$(pu')' + qu = \lambda ru \tag{1.1}$$

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and proved in a simpler way with no need of pseudoanalytic function theory (see Theorem 2.1 below). The Taylor coefficients in the SPPS representations are calculated as recursive integrals and called formal powers. The SPPS representations found numerous applications, see two recent review papers [14], [19]. In [13] SPPS representations were obtained for solutions of fourth order Sturm-Liouville equations of the form

$$(pu'')'' + (qu')' = \lambda R[u]$$

where R is a linear differential operator of the order $n \leq 3$, and in [10] for Bessel-type singular Sturm-Liouville equations. In [21] the SPPS representations were obtained for equations of the form

$$(p(x)u')' + q(x)u = \sum_{k=1}^N \lambda^k r_k(x)u$$

and used for studying spectral problems for Zakharov-Shabat systems.

In [8] it was shown that at least in the case of the one-dimensional Schrödinger equation

$$u'' + qu = \lambda u \tag{1.2}$$

the formal powers are the images of usual powers x^k , $k = 0, 1, 2, \dots$ under the action of a corresponding transmutation operator. In [20] based on this observation a new method for solving spectral problems for (1.2) was developed. The method possesses a remarkable unique feature: it allows one to compute thousands of eigendata with a non-decreasing accuracy. In [9], [7], [8] and [15] methods for solving different problems for partial differential equations involving the computation of formal powers were developed.

Thus, the computation of formal powers is required for application of different methods and in different models. An important restriction for computing formal powers as proposed in [16], [18] and further publications consisted in the necessity of a nonvanishing particular solution of the equation

$$(pv')' + qv = 0. \tag{1.3}$$

When p and q are real valued (and sufficiently regular) such nonvanishing solution can be proposed in the form $v_0 = v_1 + iv_2$ where v_1 and v_2 are arbitrary linearly independent real-valued solutions of (1.3). However for complex-valued coefficients p and q there is no such simple way for its construction. Moreover, even when v_0 does not vanish but in some points is relatively close to zero, the computation of formal powers may present difficulties.

In the present work we solve two problems. 1) We develop an SPPS representation which is not limited to nonvanishing particular solutions of auxiliary equations and admits certain “nastiness” in the coefficients. For example, p is allowed to have zeros. 2) We extend the SPPS method onto equations of the form

$$(p(x)u')' + q(x)u = \sum_{k=1}^N \lambda^k R_k[u], \quad x \in (a, b) \tag{1.4}$$

where $R_k[u] := r_k(x)u + s_k(x)u'$, $k = 1, \dots, N$, the complex-valued functions p , q , r_k , s_k are continuous on the finite segment $[a, b]$. The presented numerical results show that nowadays this is one of the most accurate ways for solving corresponding spectral problems with a wide range of applicability (e.g., few available algorithms are applicable to complex coefficients, complex spectra, polynomial pencils of operators, etc.).

In Section 2 we prove new relations concerning formal powers and obtain the modified SPPS representations for Sturm-Liouville equations of the form (1.1). In Section 3 we extend this result onto equations of the form (1.4). In Section 4 we describe the algorithm and the numerical implementation of the proposed method for solving spectral problems and give eight numerical examples illustrating its performance.

2 SPPS representations

2.1 The original SPPS representation

In [18] the following theorem was proved.

Theorem 2.1 (SPPS representation, [18]). Assume that on a finite segment $[a, b]$, equation

$$(pv')' + qv = 0, \quad (2.1)$$

possesses a particular solution f such that the functions $f^2 r$ and $1/(f^2 p)$ are continuous on $[a, b]$. Then the general solution of the equation

$$(pu')' + qu = \lambda ru \quad (2.2)$$

on (a, b) has the form

$$u = c_1 u_1 + c_2 u_2 \quad (2.3)$$

where c_1 and c_2 are arbitrary complex constants,

$$u_1 = f \sum_{k=0}^{\infty} \lambda^k \tilde{X}^{(2k)} \quad \text{and} \quad u_2 = f \sum_{k=0}^{\infty} \lambda^k X^{(2k+1)} \quad (2.4)$$

with $\tilde{X}^{(n)}$ and $X^{(n)}$ being defined by the recursive relations $\tilde{X}^{(-n)} \equiv X^{(-n)} \equiv 0$ for $n \in \mathbb{N}$,

$$\tilde{X}^{(0)} \equiv 1, \quad X^{(0)} \equiv 1, \quad (2.5)$$

$$\tilde{X}^{(n)}(x) = \begin{cases} \int_{x_0}^x \tilde{X}^{(n-1)}(s) f^2(s) r(s) ds, & n \text{ odd}, \\ \int_{x_0}^x \tilde{X}^{(n-1)}(s) \frac{1}{f^2(s)p(s)} ds, & n \text{ even}, \end{cases} \quad (2.6)$$

$$X^{(n)}(x) = \begin{cases} \int_{x_0}^x X^{(n-1)}(s) \frac{1}{f^2(s)p(s)} ds, & n \text{ odd}, \\ \int_{x_0}^x X^{(n-1)}(s) f^2(s) r(s) ds, & n \text{ even}, \end{cases} \quad (2.7)$$

where x_0 is an arbitrary point in $[a, b]$ such that p is continuous at x_0 and $p(x_0) \neq 0$. Further, both series in (2.4) converge uniformly on $[a, b]$.

The solutions u_1 and u_2 satisfy the initial conditions

$$\begin{aligned} u_1(x_0) &= f(x_0), & u_1'(x_0) &= f'(x_0), \\ u_2(x_0) &= 0, & u_2'(x_0) &= \frac{1}{f(x_0)p(x_0)}. \end{aligned}$$

This result was first obtained in [16] with the aid of pseudoanalytic function theory [17] and for the case $r \equiv 1$. The functions $\tilde{X}^{(n)}$ and $X^{(n)}$ are called *formal powers* since they generalize the usual powers $(x - x_0)^n$ or more precisely $(x - x_0)^n/n!$ (when $f \equiv p \equiv r \equiv 1$).

2.2 Relations between formal powers associated with two different particular solutions

Now let us suppose additionally that $f(x_0) = 1$ and that together with f there exists another linearly independent solution g of (2.1) satisfying the same conditions as f and such that $g(x_0) = 1$. Then one can construct formal powers corresponding to g . Let us denote them by $\tilde{Y}^{(n)}$ and $Y^{(n)}$ correspondingly. Thus, $\tilde{Y}^{(-n)} \equiv Y^{(-n)} \equiv 0$ for $n \in \mathbb{N}$,

$$\begin{aligned} \tilde{Y}^{(0)} &\equiv 1, & Y^{(0)} &\equiv 1, \\ \tilde{Y}^{(n)}(x) &= \begin{cases} \int_{x_0}^x \tilde{Y}^{(n-1)}(s) g^2(s) r(s) ds, & n \text{ odd}, \\ \int_{x_0}^x \tilde{Y}^{(n-1)}(s) \frac{1}{g^2(s)p(s)} ds, & n \text{ even}, \end{cases} \\ Y^{(n)}(x) &= \begin{cases} \int_{x_0}^x Y^{(n-1)}(s) \frac{1}{g^2(s)p(s)} ds, & n \text{ odd}, \\ \int_{x_0}^x Y^{(n-1)}(s) g^2(s) r(s) ds, & n \text{ even}. \end{cases} \end{aligned}$$

Later on we will show that the restrictions imposed on f and g can be relaxed. At this moment we need them to establish relations between the two sets of formal powers. Denote $\rho = \frac{1}{p(x_0)(g'(x_0) - f'(x_0))}$.

Proposition 2.2. *Assume that on a finite interval $[a, b]$, equation (2.1) possesses two particular solutions f and g such that $f(x_0) = g(x_0) = 1$, x_0 is an arbitrary point in $[a, b]$ such that p is continuous at x_0 and $p(x_0) \neq 0$, the functions $f^2 r$, $1/(f^2 p)$, $g^2 r$ and $1/(g^2 p)$ are continuous on $[a, b]$. Then the following relations hold*

$$gY^{(2k+1)} = fX^{(2k+1)} \quad (2.8)$$

$$= \rho(g\tilde{Y}^{(2k)} - f\tilde{X}^{(2k)}) \quad (2.9)$$

$$= \rho(gX^{(2k)} - fY^{(2k)}), \quad (2.10)$$

$$g\tilde{Y}^{(2k)} = gX^{(2k)} + \rho(g\tilde{X}^{(2k-1)} - f\tilde{Y}^{(2k-1)}), \quad (2.11)$$

$$f\tilde{X}^{(2k)} = fY^{(2k)} + \rho(g\tilde{X}^{(2k-1)} - f\tilde{Y}^{(2k-1)}) \quad (2.12)$$

for any $k = 0, 1, 2, \dots$

Proof. Consider two pairs of linearly independent solutions of (2.2) constructed according to Theorem 2.1. One pair is generated by the particular solution f and has the form (2.4) meanwhile the second pair is generated by g and has the form

$$v_1 = g \sum_{k=0}^{\infty} \lambda^k \tilde{Y}^{(2k)} \quad \text{and} \quad v_2 = g \sum_{k=0}^{\infty} \lambda^k Y^{(2k+1)}.$$

Due to Theorem 2.1 the solutions v_1 and v_2 satisfy the initial conditions $v_1(x_0) = g(x_0)$, $v_1'(x_0) = g'(x_0)$, $v_2(x_0) = 0$, $v_2'(x_0) = \frac{1}{g(x_0)p(x_0)}$. Since $f(x_0) = g(x_0) = 1$, we obtain $u_2 \equiv v_2$. From the equality of the corresponding series (2.4) for any value of the parameter λ we obtain (2.8).

Comparison of the initial conditions gives us also the following relation

$$v_1 = u_1 + \frac{1}{\rho} u_2.$$

Thus,

$$g \sum_{k=0}^{\infty} \lambda^k \tilde{Y}^{(2k)} = f \sum_{k=0}^{\infty} \lambda^k \tilde{X}^{(2k)} + \frac{1}{\rho} f \sum_{k=0}^{\infty} \lambda^k X^{(2k+1)}$$

for any $\lambda \in \mathbb{C}$. Hence for any $k = 0, 1, 2, \dots$ we have

$$g\tilde{Y}^{(2k)} = f \left(\tilde{X}^{(2k)} + \frac{1}{\rho} X^{(2k+1)} \right)$$

from where (2.9) follows.

Consider the equality $u_2' \equiv v_2'$. It implies the equality of the series

$$f' \sum_{k=0}^{\infty} \lambda^k X^{(2k+1)} + \frac{1}{fp} \sum_{k=0}^{\infty} \lambda^k X^{(2k)} = g' \sum_{k=0}^{\infty} \lambda^k Y^{(2k+1)} + \frac{1}{gp} \sum_{k=0}^{\infty} \lambda^k Y^{(2k)}$$

and hence

$$f' X^{(2k+1)} + \frac{1}{fp} X^{(2k)} = g' Y^{(2k+1)} + \frac{1}{gp} Y^{(2k)}$$

for any $k = 0, 1, 2, \dots$. From (2.8) we have $g' Y^{(2k+1)} = \frac{g'}{g} f X^{(2k+1)}$ and consequently,

$$\left(f' - \frac{g'}{g} f \right) X^{(2k+1)} = \frac{1}{p} \left(\frac{1}{g} Y^{(2k)} - \frac{1}{f} X^{(2k)} \right).$$

Notice that by Liouville's formula for the Wronskian

$$g'f - gf' = W(f, g) = \frac{p(x_0)}{p} W(f, g)(x_0) = \frac{1}{\rho p}. \quad (2.13)$$

Then

$$\frac{1}{\rho} X^{(2k+1)} = \frac{g}{f} X^{(2k)} - Y^{(2k)}$$

from where we obtain (2.10).

Consider the equality $v'_1 = u'_1 + \frac{1}{\rho} u'_2$. It can be written in the form

$$\begin{aligned} g' \sum_{k=0}^{\infty} \lambda^k \tilde{Y}^{(2k)} + \frac{1}{gp} \sum_{k=1}^{\infty} \lambda^k \tilde{Y}^{(2k-1)} &= f' \sum_{k=0}^{\infty} \lambda^k \tilde{X}^{(2k)} + \frac{1}{fp} \sum_{k=1}^{\infty} \lambda^k \tilde{X}^{(2k-1)} \\ &+ \frac{1}{\rho} \left(f' \sum_{k=0}^{\infty} \lambda^k X^{(2k+1)} + \frac{1}{fp} \sum_{k=0}^{\infty} \lambda^k X^{(2k)} \right) \end{aligned}$$

which leads to the equality

$$g' \tilde{Y}^{(2k)} + \frac{1}{gp} \tilde{Y}^{(2k-1)} = f' \tilde{X}^{(2k)} + \frac{1}{fp} \tilde{X}^{(2k-1)} + \frac{1}{\rho} \left(f' X^{(2k+1)} + \frac{1}{fp} X^{(2k)} \right)$$

for any $k = 0, 1, 2, \dots$. Using (2.9) we obtain

$$g' \tilde{Y}^{(2k)} + \frac{1}{gp} \tilde{Y}^{(2k-1)} = \frac{1}{fp} \tilde{X}^{(2k-1)} + \frac{f'g}{f} \tilde{Y}^{(2k)} + \frac{1}{\rho fp} X^{(2k)}.$$

Thus,

$$\left(g' - \frac{f'}{f} g \right) \tilde{Y}^{(2k)} = \frac{1}{p} \left(\frac{1}{f} \tilde{X}^{(2k-1)} - \frac{1}{g} \tilde{Y}^{(2k-1)} + \frac{1}{\rho f} X^{(2k)} \right),$$

and taking into account (2.13) we arrive at (2.11). Finally, (2.12) is the same (2.11) where g plays the role of f and vice versa. ■

2.3 Modified SPSP representation

The relations between formal powers established in Proposition 2.2 suggest another way for defining the formal powers and formulating the SPSP representations for solutions of the Sturm-Liouville equation.

Definition 2.3. Let equation (2.1) admit two linearly independent solutions f and g such that $\{f, g, pf', pg'\} \subset C^1[a, b]$ and $f(x_0) = g(x_0) = 1$ where x_0 is any point of $[a, b]$ such that $p(x_0) \neq 0$. Then the following systems of functions $\{F_n\}$, $\{\tilde{F}_n\}$, $\{G_n\}$, $\{\tilde{G}_n\}$ are defined recursively as follows

$$F_{-n} \equiv G_{-n} \equiv \tilde{F}_{-n} \equiv \tilde{G}_{-n} \equiv 0 \quad \text{for } n \in \mathbb{N}, \quad (2.14)$$

$$F_0 \equiv G_0 \equiv 1, \quad \tilde{F}_0 \equiv f, \quad \tilde{G}_0 \equiv g, \quad (2.15)$$

for an odd n :

$$F_n = G_n = \rho(gF_{n-1} - fG_{n-1}), \quad (2.16)$$

$$\tilde{F}_n(x) = \int_{x_0}^x \tilde{F}_{n-1}(s) f(s) r(s) ds, \quad (2.17)$$

$$\tilde{G}_n(x) = \int_{x_0}^x \tilde{G}_{n-1}(s) g(s) r(s) ds, \quad (2.18)$$

and for an even n :

$$F_n(x) = \int_{x_0}^x F_{n-1}(s)f(s)r(s) ds, \quad (2.19)$$

$$G_n(x) = \int_{x_0}^x G_{n-1}(s)g(s)r(s) ds, \quad (2.20)$$

$$\tilde{F}_n = fG_n - \rho(f\tilde{G}_{n-1} - g\tilde{F}_{n-1}), \quad (2.21)$$

$$\tilde{G}_n = gF_n - \rho(f\tilde{G}_{n-1} - g\tilde{F}_{n-1}). \quad (2.22)$$

Notice that from (2.21) and (2.22) we have that

$$\tilde{G}_{2n} - \tilde{F}_{2n} = gF_{2n} - fG_{2n}$$

and hence from (2.16) we obtain the relation

$$F_{2n+1} = G_{2n+1} = \rho(\tilde{G}_{2n} - \tilde{F}_{2n}). \quad (2.23)$$

Remark 2.4. It is easy to see that when additionally the function $1/(f^2p)$ is continuous on $[a, b]$ and hence the systems of functions $\{X^{(n)}\}$, $\{\tilde{X}^{(n)}\}$ can be constructed, the following relations hold

$$F_n = fX^{(n)} \quad \text{and} \quad \tilde{F}_n = \tilde{X}^{(n)} \quad \text{for an odd } n$$

and

$$F_n = X^{(n)} \quad \text{and} \quad \tilde{F}_n = f\tilde{X}^{(n)} \quad \text{for an even } n.$$

In the following lemma we prove several properties of the introduced functions.

Lemma 2.5. *For the functions defined by Definition 2.3 the following relations hold.*

For an odd n :

$$F'_n = G'_n = \rho(g'F_{n-1} - f'G_{n-1}), \quad (2.24)$$

$$(pF'_n)' + qF_n = rF_{n-2}, \quad (2.25)$$

$$(pG'_n)' + qG_n = rG_{n-2}, \quad (2.26)$$

and for an even n :

$$\tilde{F}'_n = f'G_n - \rho(f'\tilde{G}_{n-1} - g'\tilde{F}_{n-1}), \quad (2.27)$$

$$\tilde{G}'_n = g'F_n - \rho(f'\tilde{G}_{n-1} - g'\tilde{F}_{n-1}), \quad (2.28)$$

$$(p\tilde{F}'_n)' + q\tilde{F}_n = r\tilde{F}_{n-2}, \quad (2.29)$$

$$(p\tilde{G}'_n)' + q\tilde{G}_n = r\tilde{G}_{n-2}. \quad (2.30)$$

Proof. Let n be odd. Then from (2.16), (2.19) and (2.20) we have $F'_n = \rho(g'F_{n-1} - f'G_{n-1}) + \rho fgr(F_{n-2} - G_{n-2})$. Due to (2.16) the difference in the last brackets equals zero and hence (2.24) holds.

Consider $(pF'_n)' = \rho((pg')'F_{n-1} - (pf')'G_{n-1} + pr(g'fF_{n-2} - f'gG_{n-2}))$. Now from (2.16), (2.13) and the fact that f and g are solutions of (2.1) we obtain $(pF'_n)' = -q\rho(gF_{n-1} - fG_{n-1}) + rF_{n-2}$ and hence (2.25). Equality (2.26) is proved similarly.

Let n be even. Differentiating (2.21) and using (2.17), (2.18) and (2.20) we obtain

$$\tilde{F}'_n = f'G_n + fgrG_{n-1} - \rho(f'\tilde{G}_{n-1} - g'\tilde{F}_{n-1}) - \rho fgr(\tilde{G}_{n-2} - \tilde{F}_{n-2}).$$

Now using (2.23) we obtain (2.27). Equality (2.28) is proved analogously. Consider

$$\begin{aligned} (p\tilde{F}'_n)' &= (pf')'G_n + pf'grG_{n-1} - \rho((pf')'\tilde{G}_{n-1} - (pg')'\tilde{F}_{n-1}) - \rho(pf'\tilde{G}'_{n-1} - pg'\tilde{F}'_{n-1}) \\ &= -qfG_n + pf'grG_{n-1} - q\rho(g\tilde{F}_{n-1} - f\tilde{G}_{n-1}) - \rho pr(f'g\tilde{G}_{n-2} - g'f\tilde{F}_{n-2}) \\ &= -q\tilde{F}_n + \rho pr(f'g(\tilde{G}_{n-2} - \tilde{F}_{n-2}) - (f'g\tilde{G}_{n-2} - g'f\tilde{F}_{n-2})) \\ &= -q\tilde{F}_n + r\tilde{F}_{n-2}. \end{aligned}$$

Thus, (2.29) is true. Equality (2.30) is proved analogously. ■

Lemma 2.6. *For the functions defined by Definition 2.3 the following inequalities hold.*

$$|F_{2k}(x)| \leq a_{2k}(c_1 c_2 c_3)^k |x - x_0|^k, \quad |G_{2k}(x)| \leq a_{2k}(c_1 c_2 c_3)^k |x - x_0|^k, \quad (2.31)$$

$$|F_{2k+1}(x)| \leq a_{2k+1} c_1 c_3 (c_1 c_2 c_3)^k |x - x_0|^k, \quad |G_{2k+1}(x)| \leq a_{2k+1} c_1 c_3 (c_1 c_2 c_3)^k |x - x_0|^k, \quad (2.32)$$

$$|\tilde{F}_{2k}(x)| \leq b_{2k} c_3 (c_1 c_2 c_3)^k |x - x_0|^k, \quad |\tilde{G}_{2k}(x)| \leq b_{2k} c_3 (c_1 c_2 c_3)^k |x - x_0|^k, \quad (2.33)$$

$$|\tilde{F}_{2k+1}(x)| \leq b_{2k+1} c_2 c_3 (c_1 c_2 c_3)^k |x - x_0|^{k+1}, \quad |\tilde{G}_{2k+1}(x)| \leq b_{2k+1} c_2 c_3 (c_1 c_2 c_3)^k |x - x_0|^{k+1}, \quad (2.34)$$

where $c_1 = |\rho|$, $c_2 = \max(\max_{x \in [a, b]} |fr|, \max_{x \in [a, b]} |gr|)$, $c_3 = \max(\max_{x \in [a, b]} |f|, \max_{x \in [a, b]} |g|)$, $a_{2k} = \frac{2^k}{k!}$, $a_{2k+1} = \frac{2^{k+1}}{k!}$, $b_{2k} = \frac{2^k(k+1)}{k!}$, $b_{2k+1} = \frac{2^k}{k!}$, $k = 0, 1, \dots$

Proof. For $k = 0$ all the inequalities are easily verified. Next, we assume that both inequalities (2.31) are true for some $k \in \mathbb{N}$ and consider

$$\begin{aligned} |F_{2k+1}(x)| &= |G_{2k+1}(x)| = |\rho(g(x)F_{2k}(x) - f(x)G_{2k}(x))| \leq 2a_{2k}c_1c_3(c_1c_2c_3)^k |x - x_0|^k \\ &= a_{2k+1}c_1c_3(c_1c_2c_3)^k |x - x_0|^k. \end{aligned}$$

Hence

$$|F_{2k+2}(x)| \leq \frac{a_{2k+1}}{k+1} (c_1 c_2 c_3)^{k+1} |x - x_0|^{k+1} = a_{2k+2} (c_1 c_2 c_3)^{k+1} |x - x_0|^{k+1}.$$

Thus, (2.31) and (2.32) are proved.

Now, suppose that (2.33) hold for some $k \in \mathbb{N}$. Then

$$|\tilde{F}_{2k+1}(x)| \leq b_{2k} c_2 c_3 (c_1 c_2 c_3)^k \frac{|x - x_0|^{k+1}}{k+1} = b_{2k+1} c_2 c_3 (c_1 c_2 c_3)^k |x - x_0|^{k+1}.$$

Consequently,

$$\begin{aligned} |\tilde{F}_{2k+2}(x)| &= \left| f(x)G_{2k+2}(x) + \rho(g(x)\tilde{F}_{2k+1}(x) - f(x)\tilde{G}_{2k+1}(x)) \right| \\ &\leq a_{2k+2}c_3(c_1c_2c_3)^{k+1} |x - x_0|^{k+1} + 2b_{2k+1}c_1c_2c_3^2(c_1c_2c_3)^k |x - x_0|^{k+1}. \end{aligned}$$

Notice that $b_{2k+2} = a_{2k+2} + 2b_{2k+1}$ and hence $|\tilde{F}_{2k+2}(x)| \leq b_{2k+2}c_3(c_1c_2c_3)^{k+1} |x - x_0|^{k+1}$. Thus, (2.33) and (2.34) are proved. ■

Now we are in a position to prove the SPPS representations for solutions of (2.2) in terms of the formal powers from Definition 2.3.

Theorem 2.7 (Modified SPPS representations). *Let p and q be such that there exist two linearly independent solutions f and g of equation (2.1) such that $\{f, g, pf', pg'\} \subset C^1[a, b]$ and $f(x_0) = g(x_0) = 1$ where x_0 is any point of $[a, b]$ such that $p(x_0) \neq 0$. Let r be such that $\{fr, gr\} \subset C[a, b]$. Then the general solution of (2.2) on (a, b) has the form (2.3) where*

$$u_1 = \sum_{k=0}^{\infty} \lambda^k \tilde{F}_{2k} \quad \text{and} \quad u_2 = \sum_{k=0}^{\infty} \lambda^k F_{2k+1}. \quad (2.35)$$

The derivatives of u_1 and u_2 have the form

$$pu'_1 = pf' + \sum_{k=1}^{\infty} \lambda^k (pf'G_{2k} - \rho(pf'\tilde{G}_{2k-1} - pg'\tilde{F}_{2k-1})) \quad (2.36)$$

and

$$pu'_2 = \rho \sum_{k=0}^{\infty} \lambda^k (pg'F_{2k} - pf'G_{2k}). \quad (2.37)$$

All series in (2.35)–(2.37) converge uniformly on $[a, b]$. The solutions u_1 and u_2 satisfy the initial conditions

$$u_1(x_0) = 1, \quad u'_1(x_0) = f'(x_0), \quad u_2(x_0) = 0, \quad u'_2(x_0) = \frac{1}{p(x_0)}. \quad (2.38)$$

Remark 2.8. The function p in (2.36) and (2.37) is necessary only in the case when this function possesses zeros and the derivatives f' and g' increase to infinity near the zeros of the function p . In all other cases we can easily remove all occurrences of p in (2.36) and (2.37).

Proof. Lemma 2.6 guarantees the uniform convergence of all the involved series. Moreover, it is not difficult to see that the majorizing series for $|u_1(x)|$ converges to the function $c_3(1 + c|x - x_0|)e^{c|x - x_0|}$ where $c = 2|\lambda|c_1c_2c_3$ meanwhile the majorizing series corresponding to $|u_2(x)|$ converges to $2c_1c_3e^{c|x - x_0|}$. Indeed, we have

$$|u_1(x)| \leq \sum_{k=0}^{\infty} |\lambda|^k |\tilde{F}_{2k}(x)| \leq c_3 \sum_{k=0}^{\infty} |\lambda|^k \frac{2^k(k+1)}{k!} (c_1c_2c_3)^k |x - x_0|^k.$$

Observe that $\sum_{k=0}^{\infty} \frac{(k+1)c^k}{k!} t^k = (te^{ct})' = (1 + ct)e^{ct}$. Hence

$$|u_1(x)| \leq c_3(1 + c|x - x_0|)e^{c|x - x_0|}$$

where $c = 2|\lambda|c_1c_2c_3$. Analogously we have

$$|u_2(x)| \leq 2c_1c_3e^{c|x - x_0|}.$$

Due to Lemma 2.5 we obtain that u_1 and u_2 are indeed solutions of (2.2) as well as the equalities (2.36) and (2.37).

The equalities (2.38) follow from the fact that all formal powers F_n , G_n , \tilde{F}_n and \tilde{G}_n vanish at $x = x_0$ for any $n \in \mathbb{N}$. Finally, from (2.38) it follows that u_1 and u_2 are linearly independent. ■

Remark 2.9. The requirement to know two particular solutions of equation (2.1) as well as values of their derivatives at some point in Theorem 2.7 does not present any difficulty for numerical applications, a variety of numerical methods can be used in order to construct two particular solutions, e.g., the SPPS representation can be successfully applied, see [18]. Solely the case when only one particular solution is known exactly gives some advantage to the formulas (2.5)–(2.7).

Remark 2.10. The Modified SPPS representation presented in Theorem 2.7 works not only when particular solutions are available for $\lambda_0 = 0$, but in fact when two particular solutions of the equation $(pv')' + qv = \lambda_0rv$ are known for some fixed λ_0 . The solution (2.35) now takes the form

$$u_1 = \sum_{k=0}^{\infty} (\lambda - \lambda_0)^k \tilde{F}_{2k} \quad \text{and} \quad u_2 = \sum_{k=0}^{\infty} (\lambda - \lambda_0)^k F_{2k+1}. \quad (2.39)$$

The procedure of using particular solutions at some point $\lambda_0 \neq 0$ is called the spectral shift technique.

Remark 2.11. The conditions $\{f, g, pf', pg'\} \subset C^1[a, b]$ and $\{fr, gr\} \subset C[a, b]$ in Theorem 2.7 are superfluous and are necessarily only if we are interested in the classical solutions of equation (2.2). If we allow weak solutions, the SPPS representations of the general solution (both original and modified) can be obtained under weaker assumptions on the coefficients, namely when $\{f, g, pf', pg'\} \subset AC[a, b]$ and $\{fr, gr\} \subset L^1[a, b]$. We refer the reader to [5] for further details.

Since the formal powers are the essential ingredient of several methods for solving equations and corresponding spectral problems it is important to verify whether the method of their calculation based on two particular solutions (Definition 2.3), we will call it the new method, presents computational advantages in comparison to the direct recursive integration (formulas (2.5)–(2.7)), the old method. It is clear that the new method of construction of the formal powers is applicable even when the function $1/(f^2p)$ is not necessarily continuous on $[a, b]$. For example, f and p can possess zeros on $[a, b]$. This is an important extension of applicability of the SPPS approach. Apart from it, we can highlight the following computational advantages of the new method.

1. The first several formal powers (whose contribution in the final result usually is greater than that of subsequent formal powers) are computed with a higher accuracy.
2. More formal powers can be computed. See for details [20, Examples 7.3 and 7.7].

3. Computation of formal powers is considerably more stable, especially when the particular solution f is of a larger change or nearly vanishing on the interval of interest.
4. Computation of the formal powers by the new method requires the same number of integrations as by the old method and only several more algebraic operations, i.e., the computation time essentially does not increase. In some cases the new method may be several times faster than the old one, this is due to the necessity to use complex-valued particular solution for the old method to ensure that this solution does not vanish, meanwhile for the new method one still can work with real-valued particular solutions.
5. Accuracy is much higher when the particular solution f or/and the coefficient p possess values close to zero on $[a, b]$.

Below we illustrate these points.

Example 2.12. Consider the function $f(x) = 1 + cx$ which is obviously a particular solution of the equation $f''(x) = 0$ and $f(0) = 1$. As a second particular solution of the same equation satisfying the condition $g(0) = 1$ we can choose the function $g \equiv 1$. The corresponding formal powers will be considered on the segment $[0, 10]$. It is easy to see that $G_n(x) = x^n/n!$. Moreover, due to (2.16) we have that for an odd n : $F_n(x) = x^n/n!$ meanwhile for an even n the formal powers F_n have the form $F_n(x) = \frac{x^n}{(n+1)!} (n(1+cx) + 1)$.

In a similar way the formal powers \tilde{F}_n for this example can be written down explicitly by means of Definition 2.3. All the calculations of the recursive integrals were performed in Matlab using the Newton-Cotes 6 point integration formula of 7-th order (see, e.g., [11]) with 10^5 uniformly distributed nodes. In all cases the computation took several seconds. The presented numerical results correspond to odd n , and the figures show the following difference $|x^n - n!F_n(x)| / \max_{[0,10]} x^n = |x^n - n!\tilde{F}_n(x)| / 10^n$.

First, we consider a case when f is a nice function: $c = 1$. The first few formal powers are computed more accurately by the new method meanwhile for the higher formal powers the old method resulted to be preferable. Nevertheless even in this “nice” case the error produced by the new method is not much worse than the error of the old method, see Fig. 1 (a).

Fig. 1 (b) shows that the accuracy achieved in the case of an almost vanishing function f (here $c = 0.0001 - 1/10$) is considerably better when the new method is applied.

Taking $c = 100$ one can observe on Fig. 1 (c) that the situation with the accuracy changes considerably for the old method meanwhile the new method delivers similar results as on Fig. 1 (a). Moreover, further increasing c and hence making the function f take larger values we easily arrive at a situation when the old method becomes practically useless meanwhile the new method keeps delivering accurate results. Fig. 1 (d) corresponds to $c = 1000000$.

2.4 General solution in terms of the formal powers for Darboux associated equations

Suppose that f and g are nonvanishing on a segment of interest $[a, b]$ linearly independent solutions of (2.1) such that $f(x_0) = g(x_0) = 1$, $x_0 \in [a, b]$. Then together with equation (2.2) let us consider the following Sturm-Liouville equations

$$\left(\frac{1}{r}v'\right)' + q_{1/f}v = \lambda \frac{1}{p}v \quad (2.40)$$

and

$$\left(\frac{1}{r}w'\right)' + q_{1/g}w = \lambda \frac{1}{p}w \quad (2.41)$$

where

$$q_{1/f} = -\left(\frac{q}{pr} + \frac{2}{r}\left(\frac{f'}{f}\right)^2 + \frac{f'}{fr}\frac{(pr)'}{pr}\right)$$

and $q_{1/g}$ has the same form as $q_{1/f}$ with f being replaced everywhere by g .

The functions $1/f$ and $1/g$ are solutions of (2.40) and (2.41) corresponding to $\lambda = 0$ respectively. We will call (2.40) and (2.41) the Sturm-Liouville equations Darboux associated with (2.2).

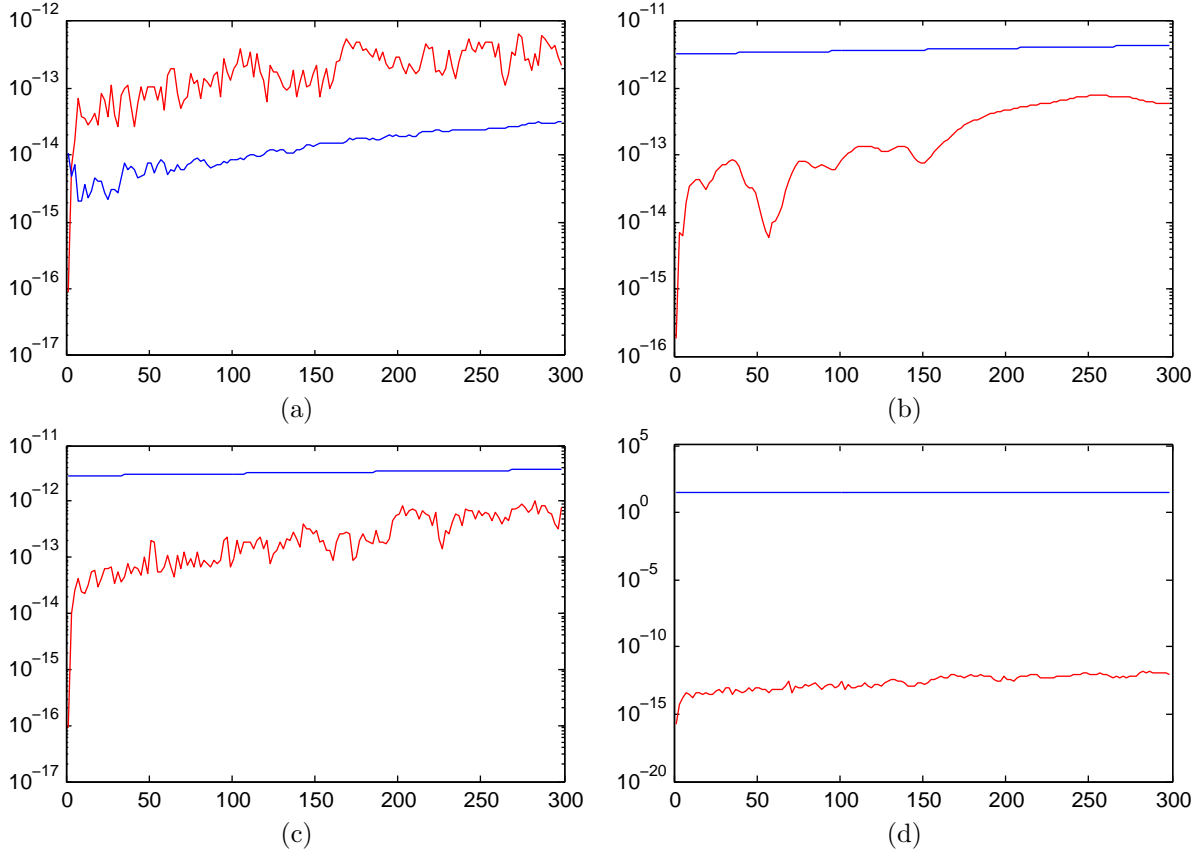


Figure 1: The blue line (which starts above) shows the error of the formal powers F_n , for odd n computed by the old method. The red line (starts below) shows the same but computed by the new method. The following values of the parameter c are used: (a) $c = 1$, (b) $c = 0.0001 - 1/10$, (c) $c = 100$ and (d) $c = 1000000$.

Let us observe that the functions

$$v_1 = \frac{1}{f} \sum_{k=0}^{\infty} \lambda^k X^{(2k)} \quad \text{and} \quad v_2 = \frac{1}{f} \sum_{k=0}^{\infty} \lambda^k \tilde{X}^{(2k+1)}$$

are linearly independent solutions of (2.40) as well as the functions

$$w_1 = \frac{1}{g} \sum_{k=0}^{\infty} \lambda^k Y^{(2k)} \quad \text{and} \quad w_2 = \frac{1}{g} \sum_{k=0}^{\infty} \lambda^k \tilde{Y}^{(2k+1)}$$

are linearly independent solutions of (2.41).

Now, from (2.35) and (2.21) we have that

$$u_1 = fg(w_1 - \lambda\rho(w_2 - v_2)), \quad (2.42)$$

and from (2.35) and (2.16),

$$u_2 = \rho fg(v_1 - w_1). \quad (2.43)$$

Equalities (2.42) and (2.43) give us expressions for the solutions of (2.2) in terms of solutions of the Darboux-associated equations (2.40) and (2.41).

Remark 2.13. The observation that for a Darboux-associated equation one has to calculate the same formal powers as for the original Sturm-Liouville equation can be used in the following way. Suppose that $1/p$ is a “nice” function meanwhile r is “nasty”, e.g., has a singularity or even an “almost” singularity, achieving

very large values. In this case one might prefer to calculate the integrals containing $1/(fp)$ in the integrand rather than those containing fr . For this it is sufficient to consider equation (2.40) and follow the described above construction beginning with Definition 2.3 where now the roles of p and r result to be interchanged.

3 SPPS representations for solutions of pencils of Sturm-Liouville operators

In this section we show that the SPPS representations analogous to those established in Theorem 2.7 can also be obtained for solutions of Sturm-Liouville equations of the form

$$(p(x)u')' + q(x)u = \sum_{k=1}^N \lambda^k R_k[u], \quad x \in (a, b) \quad (3.1)$$

where R_k are linear differential operators of the first order, $R_k[u] := r_k(x)u + s_k(x)u'$, $k = 1, \dots, N$, the complex-valued functions p, q, r_k, s_k are continuous on the finite segment $[a, b]$.

3.1 SPPS representation for solutions of pencils

It is possible to obtain the general solution of equation (3.1) by slightly changing the definition of formal powers (2.5)–(2.7). We define the formal powers for equation (3.1) as follows

$$\tilde{\mathcal{X}}^{(-n)} \equiv \mathcal{X}^{(-n)} \equiv 0 \quad \text{for } n \in \mathbb{N}, \quad (3.2)$$

$$\tilde{\mathcal{X}}^{(0)} \equiv \mathcal{X}^{(0)} \equiv 1, \quad (3.3)$$

$$\tilde{\mathcal{X}}^{(n)}(x) = \begin{cases} \int_{x_0}^x f(s) \sum_{k=1}^N R_k \left[f(s) \tilde{\mathcal{X}}^{(n-2k+1)}(s) \right] ds, & n - \text{odd}, \\ \int_{x_0}^x \tilde{\mathcal{X}}^{(n-1)}(s) \frac{ds}{f^2(s)p(s)}, & n - \text{even}, \end{cases} \quad (3.4)$$

$$\mathcal{X}^{(n)}(x) = \begin{cases} \int_{x_0}^x \mathcal{X}^{(n-1)}(s) \frac{ds}{f^2(s)p(s)}, & n - \text{odd}, \\ \int_{x_0}^x f(s) \sum_{k=1}^N R_k \left[f(s) \mathcal{X}^{(n-2k+1)}(s) \right] ds, & n - \text{even} \end{cases} \quad (3.5)$$

where x_0 is an arbitrary point of the segment $[a, b]$ such that $p(x_0) \neq 0$. The following theorem generalizes Theorem 2.1.

Theorem 3.1 (SPPS representations for polynomial pencils of operators). *Assume that on a finite interval $[a, b]$, equation (2.1) possesses a particular solution f such that the functions $fR_k[f]$, $k = 1, \dots, N$ and $\frac{1}{f^2p}$ are continuous on $[a, b]$. Then the general solution of (3.1) has the form $u = c_1u_1 + c_2u_2$, where c_1 and c_2 are arbitrary complex constants and*

$$u_1 = f \sum_{n=0}^{\infty} \lambda^n \tilde{\mathcal{X}}^{(2n)} \quad \text{and} \quad u_2 = f \sum_{n=0}^{\infty} \lambda^n \mathcal{X}^{(2n+1)}. \quad (3.6)$$

Both series in (3.6) converge uniformly on $[a, b]$.

The formulation and the proof of this theorem in the case $s_k \equiv 0$, $k = 1, \dots, N$ can be found in [21]. An analogous theorem for a perturbed Bessel equation in the case $N = 1$ can be found in [10]. The proof from [21] can be easily generalized onto the case considered here. Nevertheless we do not present here the proof of Theorem 3.1 because below we prove a stronger result generalizing Theorem 2.7 and allowing particular solution to have zeros.

3.2 Modified SPPS representation for solutions of pencils

We introduce the following definition (cf. Definition 2.3) where in order not to overload this paper with additional notations we use the same characters as above.

Definition 3.2. Let equation (2.1) admit two linearly independent solutions f and g such that $\{f, g, pf', pg'\} \subset C^1[a, b]$ and $f(x_0) = g(x_0) = 1$ where x_0 is any point of $[a, b]$ such that $p(x_0) \neq 0$. Then the following systems of functions $\{F_n\}, \{\tilde{F}_n\}, \{G_n\}, \{\tilde{G}_n\}$ are defined recursively as follows

$$\begin{aligned} F_{-n} &\equiv G_{-n} \equiv \tilde{F}_{-n} \equiv \tilde{G}_{-n} \equiv 0 & \text{for } n \in \mathbb{N}, \\ F_0 &\equiv G_0 \equiv 1, & \tilde{F}_0 \equiv f, & \tilde{G}_0 \equiv g, \end{aligned} \quad (3.7)$$

for an odd n :

$$\begin{aligned} F_n &= G_n = \rho(gF_{n-1} - fG_{n-1}), \\ \tilde{F}_n(x) &= \int_{x_0}^x f(s) \sum_{k=1}^N R_k [\tilde{F}_{n-2k+1}(s)] ds, \end{aligned} \quad (3.8)$$

$$\tilde{G}_n(x) = \int_{x_0}^x g(s) \sum_{k=1}^N R_k [\tilde{G}_{n-2k+1}(s)] ds, \quad (3.9)$$

and for an even n :

$$F_n(x) = \int_{x_0}^x f(s) \sum_{k=1}^N R_k [F_{n-2k+1}(s)] ds, \quad (3.10)$$

$$G_n(x) = \int_{x_0}^x g(s) \sum_{k=1}^N R_k [G_{n-2k+1}(s)] ds, \quad (3.11)$$

$$\begin{aligned} \tilde{F}_n &= fG_n - \rho(f\tilde{G}_{n-1} - g\tilde{F}_{n-1}), \\ \tilde{G}_n &= gF_n - \rho(f\tilde{G}_{n-1} - g\tilde{F}_{n-1}). \end{aligned}$$

From the last two equalities we have

$$\tilde{G}_{2n} - \tilde{F}_{2n} = gF_{2n} - fG_{2n}.$$

This definition may give an impression that the calculation of the formal powers involves their differentiation (application of the operators R_k under the sign of integral). Nevertheless it is easy to see that such differentiation is superfluous. Namely, we have the following equalities for the F -formal powers

$$R_k [F_{2n+1}] = \rho(R_k [g] F_{2n} - R_k [f] G_{2n}), \quad (3.12)$$

$$R_k [\tilde{F}_{2n}] = R_k [f] G_{2n} + \rho(R_k [g] \tilde{F}_{2n-1} - R_k [f] \tilde{G}_{2n-1}) \quad (3.13)$$

as well as analogous equalities for the G -formal powers G_{2n+1} and \tilde{G}_{2n} with obvious substitution of f by g and vice versa. For the proof of (3.12) it is sufficient to observe that $gF'_{2n} - fG'_{2n} = 0$. Indeed,

$$gF'_{2n} - fG'_{2n} = fg \left(\sum_{k=1}^N R_k [F_{2n-2k+1}] - \sum_{k=1}^N R_k [G_{2n-2k+1}] \right)$$

which equals zero because every operator R_k is linear and $F_{2n-2k+1} \equiv G_{2n-2k+1}$ by definition. Equality (3.13) is proved in a similar way.

Thus, for a practical use of Definition 3.2 instead of (3.8) and (3.9) it is convenient to use an alternative form of these equalities which does not require differentiation of formal powers

$$\tilde{F}_{2n+1}(x) = \int_{x_0}^x f(s) \sum_{k=1}^N \left(R_k[f(s)] G_{2n-2k+2}(s) + \rho(R_k[g(s)] \tilde{F}_{2n-2k+1}(s) - R_k[f(s)] \tilde{G}_{2n-2k+1}(s)) \right) ds, \quad (3.14)$$

$$\tilde{G}_{2n+1}(x) = \int_{x_0}^x g(s) \sum_{k=1}^N \left(R_k[g(s)] F_{2n-2k+2}(s) + \rho(R_k[g(s)] \tilde{F}_{2n-2k+1}(s) - R_k[f(s)] \tilde{G}_{2n-2k+1}(s)) \right) ds, \quad (3.15)$$

and analogously, instead of (3.10) and (3.11) their alternative form

$$F_{2n}(x) = \rho \int_{x_0}^x f(s) \sum_{k=1}^N (R_k[g(s)] F_{2n-2k}(s) - R_k[f(s)] G_{2n-2k}(s)) ds, \quad (3.16)$$

$$G_{2n}(x) = \rho \int_{x_0}^x g(s) \sum_{k=1}^N (R_k[g(s)] F_{2n-2k}(s) - R_k[f(s)] G_{2n-2k}(s)) ds. \quad (3.17)$$

Lemma 3.3. *For the functions defined by Definition 3.2 the following relations hold.
For an odd n :*

$$\begin{aligned} F'_n &= G'_n = \rho(g'F_{n-1} - f'G_{n-1}), \\ (pF'_n)' + qF_n &= \sum_{k=1}^N R_k[F_{n-2k}], \\ (pG'_n)' + qG_n &= \sum_{k=1}^N R_k[G_{n-2k}], \end{aligned} \quad (3.18)$$

and for an even n :

$$\begin{aligned} \tilde{F}'_n &= f'G_n - \rho(f'\tilde{G}_{n-1} - g'\tilde{F}_{n-1}), \\ \tilde{G}'_n &= g'F_n - \rho(f'\tilde{G}_{n-1} - g'\tilde{F}_{n-1}), \\ (p\tilde{F}'_n)' + q\tilde{F}_n &= \sum_{k=1}^N R_k[\tilde{F}_{n-2k}], \\ (p\tilde{G}'_n)' + q\tilde{G}_n &= \sum_{k=1}^N R_k[\tilde{G}_{n-2k}]. \end{aligned}$$

Proof. The proof of the equalities for the first derivatives of the formal powers is completely analogous to that from Lemma 2.5. We will prove (3.18), the rest of the equalities involving second derivatives of the formal powers are proved similarly. Consider

$$(pF'_n)' = \rho((pg')'F_{n-1} - (pf')'G_{n-1}) + \rho p(g'F'_{n-1} - f'G'_{n-1}). \quad (3.19)$$

Since $p(g'F'_{n-1} - f'G'_{n-1}) = p(g'f - f'g) \sum_{k=1}^N R_k[F_{n-2k}] = \frac{1}{\rho} \sum_{k=1}^N R_k[F_{n-2k}]$, from (3.19) we have

$$(pF'_n)' = -\rho q(gF_{n-1} - fG_{n-1}) + \sum_{k=1}^N R_k[F_{n-2k}]$$

which is (3.18). ■

Lemma 3.4. Let $c_1 = |\rho|$, $c_2 = \max_{k=1, \dots, N} (\max_{x \in [a, b]} |R_k[f]|, \max_{x \in [a, b]} |R_k[g]|)$ and $c_3 = \max(\max_{x \in [a, b]} |f|, \max_{x \in [a, b]} |g|)$. Then for the functions defined by Definition 3.2 the following inequalities hold.

$$|F_{2n}(x)| \leq \sum_{k=0}^{n - \lfloor \frac{n}{N} \rfloor} \binom{n}{k} \frac{(2c_1 c_2 c_3)^{n-k} |x - x_0|^{n-k}}{(n-k)!}, \quad (3.20)$$

$$|G_{2n}(x)| \leq \sum_{k=0}^{n - \lfloor \frac{n}{N} \rfloor} \binom{n}{k} \frac{(2c_1 c_2 c_3)^{n-k} |x - x_0|^{n-k}}{(n-k)!} \quad (3.21)$$

$$|F_{2n+1}(x)| = |G_{2n+1}(x)| \leq 2c_1 c_3 \sum_{k=0}^{n - \lfloor \frac{n}{N} \rfloor} \binom{n}{k} \frac{(2c_1 c_2 c_3)^{n-k} |x - x_0|^{n-k}}{(n-k)!}, \quad (3.22)$$

$$|\tilde{F}_{2n}(x)| \leq c_3 \sum_{k=0}^{n - \lfloor \frac{n}{N} \rfloor} \binom{n}{k} \frac{(2c_1 c_2 c_3)^{n-k} |x - x_0|^{n-k} (n-k+1)}{(n-k)!}, \quad (3.23)$$

$$|\tilde{G}_{2n}(x)| \leq c_3 \sum_{k=0}^{n - \lfloor \frac{n}{N} \rfloor} \binom{n}{k} \frac{(2c_1 c_2 c_3)^{n-k} |x - x_0|^{n-k} (n-k+1)}{(n-k)!}, \quad (3.24)$$

$$|\tilde{F}_{2n+1}(x)| \leq c_2 c_3 \sum_{k=0}^{n+1 - \lfloor \frac{n+1}{N} \rfloor} \binom{n+1}{k} \frac{(2c_1 c_2 c_3)^{n-k} |x - x_0|^{n+1-k}}{(n-k)!}, \quad (3.25)$$

$$|\tilde{G}_{2n+1}(x)| \leq c_2 c_3 \sum_{k=0}^{n+1 - \lfloor \frac{n+1}{N} \rfloor} \binom{n+1}{k} \frac{(2c_1 c_2 c_3)^{n-k} |x - x_0|^{n+1-k}}{(n-k)!}, \quad (3.26)$$

where $\lfloor x \rfloor$ denotes the largest integer less than or equal to x .

Remark 3.5. In the case when $N = 1$ and $s_1 \equiv 0$, the estimates (3.20)–(3.26) coincide with the estimates given in Lemma 2.6.

Proof. Clearly inequalities (3.20) and (3.21) hold for $n = 0$. Assume that inequalities (3.20) and (3.21) hold for all n , $0 \leq n < m$ for some $m \in \mathbb{N}$. Then taking into account (3.7) we obtain from (3.16) that

$$\begin{aligned} |F_{2m}(x)| &= \left| \rho \int_{x_0}^x f(s) \sum_{j=1}^{\min(N, m)} (R_j[g(s)] F_{2m-2j}(s) - R_j[f(s)] G_{2m-2j}(s)) ds \right| \\ &\leq 2c_1 c_2 c_3 \sum_{j=1}^{\min(N, m)} \int_{x_0}^x \sum_{k=0}^{m-j - \lfloor \frac{m-j}{N} \rfloor} \binom{m-j}{k} \frac{(2c_1 c_2 c_3)^{m-j-k} |x - x_0|^{m-j-k}}{(m-j-k)!} ds \\ &= \sum_{j=1}^{\min(N, m)} \sum_{k=0}^{m-j - \lfloor \frac{m-j}{N} \rfloor} \binom{m-j}{k} \frac{(2c_1 c_2 c_3)^{m-j-k+1} |x - x_0|^{m-j-k+1}}{(m-j-k+1)!}. \end{aligned}$$

We rearrange the terms with respect to $\ell = k + j - 1$. It follows from $1 \leq j \leq \min(N, m)$ and $0 \leq k \leq m - j - \lfloor \frac{m-j}{N} \rfloor$ that $0 \leq \ell \leq m - 1 - \lfloor \frac{m-j}{N} \rfloor \leq m - 1 - \lfloor \frac{m-N}{N} \rfloor = m - \lfloor \frac{m}{N} \rfloor$ and that $j \leq \min(N, m, \ell + 1)$. Hence

$$\begin{aligned} |F_{2m}(x)| &\leq \sum_{\ell=0}^{m - \lfloor \frac{m}{N} \rfloor} \sum_{j=1}^{\min(N, m, \ell+1)} \binom{(m-1) - (j-1)}{\ell - (j-1)} \frac{(2c_1 c_2 c_3)^{m-\ell} |x - x_0|^{m-\ell}}{(m-\ell)!} \\ &\leq \sum_{\ell=0}^{m - \lfloor \frac{m}{N} \rfloor} \frac{(2c_1 c_2 c_3)^{m-\ell} |x - x_0|^{m-\ell}}{(m-\ell)!} \sum_{j=0}^{\ell} \binom{m-1-j}{\ell-j} = \sum_{\ell=0}^{m - \lfloor \frac{m}{N} \rfloor} \binom{m}{\ell} \frac{(2c_1 c_2 c_3)^{m-\ell} |x - x_0|^{m-\ell}}{(m-\ell)!}. \end{aligned}$$

Similarly we obtain inequality (3.21). Now (3.22) easily follows from the definition.

It is easy to see from (3.14), (3.15) that inequalities (3.25) and (3.26) hold for $n = 0$. Assume that inequalities (3.25) and (3.26) hold for all n , $0 \leq n < m$. Similarly to the first part of the proof we obtain from (3.14) that

$$\begin{aligned}
|\tilde{F}_{2m+1}(x)| &\leq \sum_{j=1}^{\min(N, m+1)} c_2 c_3 \sum_{k=0}^{m+1-j-\lceil \frac{m+1-j}{N} \rceil} \binom{m+1-j}{k} \frac{(2c_1 c_2 c_3)^{m-j-k+1} |x-x_0|^{m-j-k+2}}{(m-j-k+2)!} \\
&\quad + \sum_{j=1}^{\min(N, m)} 2c_1 c_2 c_3 \cdot c_2 c_3 \sum_{k=0}^{m+1-j-\lceil \frac{m+1-j}{N} \rceil} \binom{m+1-j}{k} \frac{(2c_1 c_2 c_3)^{m-j-k} |x-x_0|^{m-j-k+2}}{(m-j-k+2) \cdot (m-j-k)!} \\
&\leq c_2 c_3 \sum_{j=1}^{\min(N, m+1)} \sum_{k=0}^{m+1-j-\lceil \frac{m+1-j}{N} \rceil} \binom{m+1-j}{k} \frac{(2c_1 c_2 c_3)^{m-j-k+1} |x-x_0|^{m-j-k+2}}{(m-j-k+1)!},
\end{aligned}$$

end the proof can be finished as in the first part.

Now inequalities (3.23) and (3.24) easily follow from the definition. ■

The following corollary presents rougher estimates than those in Lemma 3.4 however better suited for the convergency testing.

Corollary 3.6. *Under the conditions of Lemma 3.4 define*

$$C(n, x) := \frac{(1 + 2c_1 c_2 c_3 |x - x_0|)^n}{\left(\left\lceil \frac{n}{N} \right\rceil\right)!}.$$

Then for the functions F_n , \tilde{F}_n , $n \geq 0$, the following estimates hold.

$$\begin{aligned}
|F_{2n}(x)| &\leq C(n, x), & |F_{2n+1}(x)| &\leq 2c_1 c_3 C(n, x), \\
|\tilde{F}_{2n}(x)| &\leq (n+1)c_3 C(n, x), & |\tilde{F}_{2n+1}(x)| &\leq \frac{n+1}{2c_1} C(n+1, x).
\end{aligned}$$

The same estimates hold for the functions G_n , \tilde{G}_n .

Proof. Consider the inequality (3.25). We have $n+1-k \geq \lceil \frac{n+1}{N} \rceil$ hence

$$\begin{aligned}
|\tilde{F}_{2n+1}(x)| &\leq \frac{1}{2c_1} \sum_{k=0}^{n+1-\lceil \frac{n+1}{N} \rceil} \binom{n+1}{k} \frac{(n+1-k)(2c_1 c_2 c_3)^{n+1-k} |x-x_0|^{n+1-k}}{(n+1-k)!} \\
&\leq \frac{n+1}{2c_1 \left(\left\lceil \frac{n+1}{N} \right\rceil\right)!} \sum_{k=0}^{n+1-\lceil \frac{n+1}{N} \rceil} \binom{n+1}{k} (2c_1 c_2 c_3)^{n+1-k} |x-x_0|^{n+1-k} \leq \frac{n+1}{2c_1} C(n+1, x).
\end{aligned}$$

Other inequalities can be obtained similarly. ■

Theorem 3.7 (Modified SPPS representations for Sturm-Liouville pencils). *Let p and q be such that there exist two linearly independent solutions f and g of equation (2.1) such that $\{f, g, pf', pg'\} \subset C^1[a, b]$ and $f(x_0) = g(x_0) = 1$ where x_0 is any point of $[a, b]$ such that $p(x_0) \neq 0$. Let the operators R_k in (3.1) be such that $\{R_k[f], R_k[g]\} \subset C[a, b]$, $k = \overline{1, N}$. Then the general solution of (3.1) on (a, b) has the form (2.3) where*

$$u_1 = \sum_{n=0}^{\infty} \lambda^n \tilde{F}_{2n} \quad \text{and} \quad u_2 = \sum_{n=0}^{\infty} \lambda^n F_{2n+1}. \quad (3.27)$$

The derivatives of u_1 and u_2 have the form

$$pu'_1 = pf' + \sum_{n=1}^{\infty} \lambda^n \left(pf' G_{2n} - \rho(pf' \tilde{G}_{2n-1} - pg' \tilde{F}_{2n-1}) \right) \quad (3.28)$$

and

$$pu'_2 = \rho \sum_{n=0}^{\infty} \lambda^n (pg'F_{2n} - pf'G_{2n}). \quad (3.29)$$

All series in (3.27)–(3.29) converge uniformly on $[a, b]$ (see also Remark 2.8). The solutions u_1 and u_2 satisfy the initial conditions

$$u_1(x_0) = 1, \quad u'_1(x_0) = f'(x_0), \quad u_2(x_0) = 0, \quad u'_2(x_0) = \frac{1}{p(x_0)}. \quad (3.30)$$

Proof. Corollary 3.6 guarantees the uniform convergence of all the involved series. For example, we have

$$\begin{aligned} |u_2| &\leq \sum_{n=0}^{\infty} |\lambda|^n |F_{2n+1}| \leq 2c_1c_3 \sum_{n=0}^{\infty} \frac{(1 + 2c_1c_2c_3|x - x_0|)^n |\lambda|^n}{\left(\left[\frac{n}{N}\right]\right)!} \\ &= 2c_1c_3 \left(\sum_{n=0}^{N-1} M^n\right) \sum_{m=0}^{\infty} \frac{M^{mN}}{m!} = 2c_1c_3 \left(\sum_{n=0}^{N-1} M^n\right) \exp(M^N), \end{aligned}$$

where $M = (1 + 2c_1c_2c_3|x - x_0|)|\lambda|$.

Due to Lemma 3.3 we obtain that u_1 and u_2 are indeed solutions of (3.1) as well as the equalities (3.28) and (3.29). Indeed, let us consider application of the operator L to u_1 ,

$$L \left[\sum_{n=0}^{\infty} \lambda^n \tilde{F}_{2n} \right] = \sum_{n=0}^{\infty} \lambda^n \sum_{k=1}^N R_k \left[\tilde{F}_{2n-2k} \right] = \sum_{k=1}^N \lambda^k R_k \left[\sum_{n=0}^{\infty} \lambda^{n-k} \tilde{F}_{2n-2k} \right].$$

Taking into account that the formal powers with negative subindices equal zero we obtain that u_1 satisfies (3.1). For u_2 the proof is analogous.

The equalities (2.38) follow from the fact that all formal powers F_n , G_n , \tilde{F}_n and \tilde{G}_n vanish at $x = x_0$ for any $n \in \mathbb{N}$. Finally, from (2.38) it follows that u_1 and u_2 are linearly independent. ■

3.3 Spectral shift for pencils

Let λ_0 be a fixed complex number and $\lambda = \lambda_0 + \Lambda$. The right hand side of equation (3.1) can be written in the form

$$\begin{aligned} \sum_{k=1}^N \lambda^k R_k[u] &= \sum_{k=1}^N R_k[u] \sum_{\ell=0}^k \binom{k}{\ell} \lambda_0^\ell \Lambda^{k-\ell} \\ &= \sum_{k=1}^N \lambda_0^k R_k[u] + \sum_{k=1}^N \Lambda^k \sum_{\ell=0}^{N-k} \binom{k+\ell}{\ell} \lambda_0^\ell R_{k+\ell}[u], \end{aligned}$$

therefore equation (3.1) can be transformed into equation

$$L_0 u = \sum_{k=1}^N \Lambda^k \sum_{\ell=0}^{N-k} \binom{k+\ell}{\ell} \lambda_0^\ell R_{k+\ell}[u], \quad (3.31)$$

where

$$L_0 u = (pu')' + qu - \sum_{k=1}^N \lambda_0^k R_k[u] = (pu')' + u \left(q - \sum_{k=1}^N \lambda_0^k r_k \right) - u' \sum_{k=1}^N \lambda_0^k s_k.$$

Equation (3.31) is of the form (3.1) only for some special cases, say all the coefficients s_k are identically zeros or the coefficients s_k are linearly dependent and such that for some special values of λ_0 the expression $\sum_{k=1}^N \lambda_0^k s_k$ equals zero. In other situations equation (3.31) has nonzero coefficient near u' . To overcome this difficulty we multiply all terms of equation (3.31) by

$$P(x) := \exp \left(- \int_{x_0}^x \frac{1}{p(s)} \sum_{k=1}^N \lambda_0^k s_k(s) ds \right),$$

and transform it into the equation

$$(\tilde{p}u')' + \tilde{q}u = \sum_{k=1}^N \Lambda^k \tilde{R}_k[u], \quad (3.32)$$

where

$$\tilde{p} = p \cdot P, \quad \tilde{q} = P \left(q - \sum_{k=1}^N \lambda_0^k r_k \right) \quad (3.33)$$

and

$$\tilde{R}_k[u] = \tilde{r}_k u + \tilde{s}_k u' \quad \text{with} \quad \tilde{r}_k = P \cdot \sum_{\ell=0}^{N-k} \binom{k+\ell}{\ell} \lambda_0^\ell r_{k+\ell}, \quad \tilde{s}_k = P \cdot \sum_{\ell=0}^{N-k} \binom{k+\ell}{\ell} \lambda_0^\ell s_{k+\ell}. \quad (3.34)$$

Note that a particular solution of (3.32) corresponding to $\Lambda = 0$ is the particular solution of (3.1) corresponding to $\lambda = \lambda_0$. Hence applying Theorem 3.7 to equation (3.32) and taking into account that $\tilde{p}(x_0) = p(x_0)$ we obtain the following corollary.

Corollary 3.8 (Spectral shift for the modified SPPS representation). *Let equation (3.1) admit for $\lambda = \lambda_0$ two linearly independent solutions f and g such that $\{f, g, pf', pg'\} \subset C^1[a, b]$ and $f(x_0) = g(x_0) = 1$ where x_0 is any point of $[a, b]$ such that $p(x_0) \neq 0$. Let $\frac{1}{p} \sum_{k=1}^N \lambda_0^k s_k \in C[a, b]$ and $\{R_k[f], R_k[g]\} \subset C[a, b]$, $k = \overline{1, N}$. Then the general solution of (3.1) on (a, b) has the form (2.3) where*

$$u_1 = \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n \tilde{F}_{2n} \quad \text{and} \quad u_2 = \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n F_{2n+1}, \quad (3.35)$$

and the functions $\{F_n\}$ and $\{\tilde{F}_n\}$ are obtained by applying formulas from Definition 3.2 to the functions f , g and $\tilde{R}_k[f]$, $\tilde{R}_k[g]$.

The derivatives of u_1 and u_2 have the form

$$pu'_1 = pf' + \sum_{n=1}^{\infty} (\lambda - \lambda_0)^n \left(pf' G_{2n} - \rho(pf' \tilde{G}_{2n-1} - pg' \tilde{F}_{2n-1}) \right) \quad (3.36)$$

and

$$pu'_2 = \rho \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n (pg' F_{2n} - pf' G_{2n}). \quad (3.37)$$

All series in (3.35)–(3.37) converge uniformly on $[a, b]$. The solutions u_1 and u_2 satisfy the same initial conditions (3.30).

4 Numerical solution of spectral problems

4.1 The general scheme

The general scheme of using the modified SPPS representation for the solution of spectral problems for equation (2.2) and more general (3.1) is similar to that for the original SPPS representation, see [18], [20].

Consider boundary conditions

$$\alpha_a u(a) + \beta_a p(a) u'(a) = 0 \quad (4.1)$$

$$\alpha_b u(b) + \beta_b p(b) u'(b) = 0, \quad (4.2)$$

where $\alpha_a, \beta_a, \alpha_b$ and β_b are complex numbers such that $|\alpha_a| + |\beta_a| \neq 0$ and $|\alpha_b| + |\beta_b| \neq 0$. Suppose that the function p is continuous at one of the endpoints and is different from zero at that endpoint. We may assume that a is such endpoint. Let f and g be two linearly independent solutions of (2.1) satisfying $f(a) = g(a) = 1$, and denote $h := f'(a)$. Consider the systems of functions $\{F_n\}$, $\{\tilde{F}_n\}$, $\{G_n\}$, $\{\tilde{G}_n\}$ constructed from the

solutions f and g by Definition 2.3 or by Definition 3.2 using the point $x_0 = a$. Then due to the initial conditions (2.38) or (3.30) the solution $u(x; \lambda)$ defined by

$$u(x; \lambda) = \beta_a u_1(x; \lambda) - (\alpha_a + \beta_a h) u_2(x; \lambda),$$

where the functions u_1 and u_2 are given by (2.35) or (3.27), satisfies the first boundary condition (4.1). Hence the second boundary condition (4.2) gives us the characteristic function

$$\Phi(\lambda) := \alpha_b u(b; \lambda) + \beta_b p(b) u'(b; \lambda). \quad (4.3)$$

The set of zeros of the function Φ coincides with the set of eigenvalues of the spectral problem (4.1), (4.2) for the equation (3.1). Truncating the series in (4.3) we obtain a polynomial approximating the characteristic function. The roots of this polynomial closest to zero give us approximations of the eigenvalues. The Rouché theorem guarantees that these roots are indeed the approximations to the eigenvalues and are not spurious roots appearing as a result of the truncation of the series.

In the case when the function p is not continuous or equals zero at the endpoints, we cannot calculate the formal powers starting from one of the endpoints and cannot take advantage of the initial conditions (2.38) or (3.30). Instead we consider the general solution $u = c_1 u_1 + c_2 u_2$ constructed using some point $x_0 \in (a, b)$. Then a point λ is an eigenvalue of the problem if and only if the determinant of the following system

$$\det \begin{pmatrix} \alpha_a u_1(a; \lambda) + \beta_a p(a) u'_1(a; \lambda) & \alpha_a u_2(a; \lambda) + \beta_a p(a) u'_2(a; \lambda) \\ \alpha_b u_1(b; \lambda) + \beta_b p(b) u'_1(b; \lambda) & \alpha_b u_2(b; \lambda) + \beta_b p(b) u'_2(b; \lambda) \end{pmatrix} = 0, \quad (4.4)$$

is equal to zero, see, e.g., [24, §1.3], and we can proceed as before: taking the partial sums of the involved series, obtaining a polynomial approximating the characteristic equation and choosing the roots closest to zero.

4.2 Numerical examples for Sturm-Liouville problems

In the paper [18] the authors illustrated the numerical performance of the SPPS method for solving Sturm-Liouville spectral problems. Since the difference between the original SPPS representation and the modified SPPS representation consists only in the way of calculating coefficients, the performance of the modified SPPS method is similar to that of the SPPS method when all the involved recursive integrals can be calculated equally precise. Usually it is the case when a particular solution f and functions $1/p$, r do not grow rapidly and are sufficiently separated from zero. In the opposite case one may expect a better performance of the modified SPPS method. One of the examples with a rapidly growing particular solution f , the Coffey-Evans equation, is considered in [20] where we observe that a combination of the Clenshaw-Curtis integration formula with the formulas (2.16)–(2.22) allows us to compute twice as many formal powers in comparison with the formulas (2.6), (2.7).

In this subsection we consider several “nasty” examples (according to [28, Appendix B]) involving unbounded however absolutely integrable functions $1/p$, r , q . Even though some of the problems do not satisfy the conditions of Theorem 2.7, the modified SPPS method demonstrates an excellent accuracy, meanwhile the performance of the SPPS method is considerably worse for the problems with unbounded functions $1/p$ or r . Moreover, the numerical implementation of the SPPS method is several times slower for these problems due to the necessity to use complex-valued functions in order to obtain non-vanishing particular solutions.

Example 4.1. Consider the following problem (Problem 10 from [28])

$$\begin{cases} -(\sqrt{1-x^2} u')' = \lambda u, \\ \sqrt{1-x^2} u'(x)|_{x=-1} = 0, \quad u(1) = 0, \end{cases}$$

a problem with a “nasty” $p = \sqrt{1-x^2}$ and “good” q and r .

Since the function p equals zero at both endpoints, we used the determinant approach described in the previous subsection.

The functions $f(x) = 1$ and $g(x) = 1 + \arcsin(x)$ were chosen as two particular solutions of equation (2.1) satisfying the conditions of Theorem 2.7.

n	λ_n ([28])	λ_n (our method)	λ_n (“old” SPPS method)	λ_n (SLEIGN2)
0	0.3856819	0.385681872027002	0.3863	0.385684539
1		3.80741155419017	3.8114	3.807427952
2		10.6772827352614	10.6867	10.677320922
3		20.9871308475868	21.0036	20.987197576
5		51.9221036193997	51.9570	51.922245020
10		189.421910262487	189.5241	189.422324959
15		412.863500805267	413.0592	412.864294034
20		722.245619500433	722.5567	722.246883258
24	1031.628	1031.62824937392	1032.047	1031.629950116

Table 1: The eigenvalues of the Problem 10 from [28] (Example 4.1).

We obtained approximate eigenvalues of the problem applying the spectral shift technique, on each step finding one new approximate eigenvalue as the root of the polynomial approximating the characteristic equation closest to the current spectral shift center and using this value as the spectral shift for the next step. On each step we computed $N = 100$ formal powers using machine precision arithmetics in MATLAB with $x_0 = 0$ and $M = 2 \cdot 10^5 - 1$ points for the Newton-Cotes 6 points integration scheme. We also tested the “old” SPPS method on this problem. In order to deal with the zeros of the function p at the endpoints we approximated it by a function having small, however non-zero values at the endpoints. The results from the SPPS representation were obtained using the same parameters and the strategy for the spectral shift, with the only difference that we have taken a complex-valued combination $u_1 + iu_2$ on each step for a particular solution to be non-vanishing. The obtained results are presented in Table 1 together with the values from [28] and the results produced by SLEIGN2 package [4]. Another well-known package, MATSLISE [23], can not solve this problem at all. Unfortunately the exact characteristic equation for this problem is unknown. Note that the results of the modified SPPS method are in a good agreement with those presented in [28], meanwhile the results produced by SLEIGN2 differ in 3rd–5th decimal place, the results of the SPPS method are even worse.

Example 4.2. Consider the following problem (Problem 9 from [28]). The interval is $[-1, 1]$, “nice” $p = 1/\sqrt{1-x^2}$ and $q = 0$, “nasty” $r = 1/\sqrt{1-x^2}$ with the Dirichlet boundary conditions $u(-1) = u(1) = 0$.

We tested the performance of the Darboux-associated equations approach proposed in Subsection 2.4 and Remark 2.13 on this problem. Even using the spectral shift technique, the results for the higher eigenvalues were mediocre, see Table 2. Such behavior of the method can be explained by the additional steps related with the Darboux associated equations, namely construction of the potentials $q_{1/f}$ and of a second particular solution of these associated equations. Obtained potentials $q_{1/f}$ possessed large peaks inside the interval leading to large errors in the calculated formal powers.

Additionally we applied the direct approach to check whether our method can be applied in the situations not covered by Theorem 2.7. For that we chose $f(x) = 1$ and $g(x) = 1 + (x\sqrt{1-x^2} + \arcsin x)/2$ as particular solutions of (2.1) satisfying the conditions of Theorem 2.7, changed values of r at the endpoints to be equal to some rather large values and proceeded exactly as described in Example 4.1. The obtained results are presented in Table 2 and are in an excellent agreement with those reported in [28]. Some of the eigenvalues computed by SLEIGN2 package differ from our results in 3-5th decimal place. Also we tested the performance of the SPPS method. Produced eigenvalues are closer than in the previous example to the obtained by the modified SPPS method and agree up to 4-6 decimal places.

Example 4.3. Consider the following problem (Problem 11 from [28])

$$\begin{cases} -u'' + u \ln x = \lambda u, \\ u(0) = u(4) = 0. \end{cases}$$

Again, this problem is not covered by Theorem 2.7. Nevertheless we checked the performance of our method on this problem. Two particular solutions of equation (2.1) were computed using the SPPS representation. After that we proceeded exactly as in Examples 4.1 and 4.2 using the point $x_0 = 2$ to calculate the formal powers. We also checked the performance of the SPPS method. Obtained results together with the results from [28] and the results produced by SLEIGN2 package are presented in Table 3.

n	λ_n ([28])	λ_n (our method)	λ_n (our method, based on Darboux-associated eqns.)	λ_n (SLEIGN2)
0	3.559279966	3.55927997532677	3.559280003	3.559279975351
1		12.1562946865237	12.15629481	12.15637
2		25.7034532288478	25.70345354	25.70345322896
3		44.1919717455476	44.19197235	44.19206
5		95.9831209203069	95.98312252	95.98332
9	258.8005854	258.800585373152	258.8005909	258.7976
14		573.369367026965	573.36944	573.3693670289
19		1011.31532988447	1011.19	1011.3153298853
24	1572.635284	1572.63528434735	–	1572.6352843481

Table 2: The eigenvalues of the Problem 9 from [28] (Example 4.2).

n	λ_n ([28])	λ_n (our method)	λ_n (old SPPS method)	λ_n (SLEIGN2)
0	1.1248168097	1.12481680968989	1.1248168096898	1.12481680982
1		2.99094198359879	2.99094198359867	2.990941998
2		6.03307162455419	6.03307162455413	6.03307134
4		15.8644572215756	15.8644572215752	15.86445693
9		62.0987975024207	62.0987975024165	62.0987975072
24	385.92821596	385.928215961012	385.928215961016	385.928215990

Table 3: The eigenvalues of the Problem 11 from [28] (Example 4.3).

4.3 High-precision evaluation of eigenvalues

In this subsection we show that the modified SPPS method can be successfully applied to the calculation of eigenvalues of Sturm-Liouville spectral problems with a high accuracy. However, in contrast to the method proposed in [20], the accuracy of the eigenvalues rapidly deteriorates with the eigenvalue index. The situation can be improved to some extent applying the spectral shift technique allowing one to obtain hundreds of highly accurate approximate eigenvalues.

Example 4.4. Consider the following spectral problem (the second Paine problem, [25, 28])

$$\begin{cases} -u'' + \frac{1}{(x+0.1)^2} u = \lambda u, & 0 \leq x \leq \pi, \\ u(0, \lambda) = 0, & u(\pi, \lambda) = 0. \end{cases}$$

This problem was treated in [20] and appears to be rather tough requiring a large number of formal powers to be used in order to compute highly accurate eigenvalues. In [20] we were able to achieve the accuracy of order $10^{-43} \div 10^{-42}$ almost independent of the eigenvalue index for several thousands of eigenvalues. Further increase of accuracy required significant increase of all the parameters involved (number of the formal powers, precision and the number of points used for the integration). In this example we show that the modified SPPS method allows us to improve the accuracy to the order of 10^{-150} using the similar set of parameters however only for the first 187 eigenvalues.

First we verified the precision of the coefficients of the polynomial approximating the exact characteristic function. These coefficients are nothing more than the values of the formal powers at the right endpoint divided by the corresponding factorials. We compared the different methods of indefinite numerical integration used for evaluating the formal powers. Up to now we used three different methods of indefinite numerical integration, see [10], [15] and [20]. The first is the modification of the Newton-Cotes 7th order six point rule, the second is the integration of a spline approximating a formal power and the third is the Clenshaw-Curtis integration based on the approximation of a function by the Tchebyshev polynomials. The computation time required by the second mentioned method highly exceeds the computation time required by the first method providing only a slight improvement of the accuracy. For that reason in the present work we consider only the first and the third integration methods. All the computations were performed in Wolfram Mathematica 8.

For each of the methods a parameter M corresponds to the number of smaller subdivision intervals on the segment $[0, \pi]$ used for numerical integration, i.e., the integrand function was represented by its values in $M+1$ points. For the Clenshaw-Curtis integration we used for M values 512, 1024, 2048 and 3072. For each of the values of M we computed two particular solutions using the SPPS representation and verified their precision against the exact particular solution $u_0(x) = (1 + 10x)^{(1+\sqrt{5})/2}$. The maximum absolute errors were $3.9 \cdot 10^{-85}$, $7.5 \cdot 10^{-165}$, $1.7 \cdot 10^{-323}$ and $8.2 \cdot 10^{-482}$ respectively. Therefore we used 100, 200, 400 and 600 digit arithmetic respectively for the calculation of the formal powers.

For the Newton-Cottes integration scheme we used $M = 10^4$, $5 \cdot 10^4$ and $25 \cdot 10^4$ and performed computations in machine-precision and 64-digit arithmetics, in both cases using exact particular solutions.

We compared the computed coefficients (values of the formal powers at the right endpoint divided by the corresponding factorials) against the same values produced by means of the Clenshaw-Curtis integration formula with $M = 4096$. The relative errors of the formal powers are presented on Figure 2. Note the different behavior of the errors. For the Clenshaw-Curtis integration the errors start from much lower values coinciding with the errors of the particular solutions, however rapidly increasing with the increase of the formal power number. For the Newton-Cottes integration the errors in machine-precision are almost constant and are slowly growing in the high precision arithmetic.

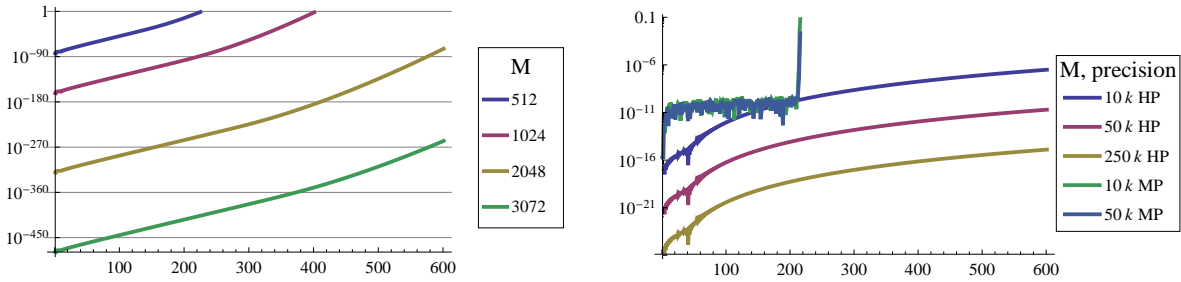


Figure 2: Relative errors of the first 600 formal powers in Example 4.4 obtained using Clenshaw-Curtis integration (on the left graph) and using the Newton-Cortes integration (on the right graph). M corresponds to the number of points used for representing the integrand, HP means 64 digit precision and MP means machine precision.

Using the obtained coefficients we calculated the roots of the polynomial approximating eigenvalues and compared them to the exact ones (see [20, Example 26] for the expression of the characteristic equation). Since the problem possesses only real eigenvalues, all roots of the polynomial having large imaginary part were discarded as spurious roots. On Figure 3 we present the graphs of the absolute errors of the approximate eigenvalues obtained from the truncation of the modified SPPS representation using $N = 100, 200, 400$ and 600 formal powers and without application of the spectral shift.

Several observations can be made regarding the presented graphs. First, the number of eigenvalues which can be approximately calculated from the truncated SPPS representation depends on the number of used formal powers and almost does not depend on the accuracy of the formal powers. Second, the accuracy of the formal powers has a great influence on the accuracy of the first eigenvalues. The errors of the first approximate eigenvalues are close to the errors achieved while calculating the particular solutions and the first several formal powers, meanwhile the errors of the larger eigenvalues remain roughly constant for different computation precisions used.

Finally we computed the approximate eigenvalues applying the spectral shift technique. We performed spectral shifts using values $\lambda_0 = 250n$, $n = 1, \dots, 200$ and on each step calculating $N = 400$ formal powers with the help of the Clenshaw-Curtis integration with $M = 1024$ and 200-digit arithmetic. The absolute errors of the first 200 found eigenvalues are presented on Figure 4. As one can see, the errors are slowly growing remaining smaller than 10^{-150} up to the eigenvalue number 186, for the higher indices the accuracy rapidly deteriorates.

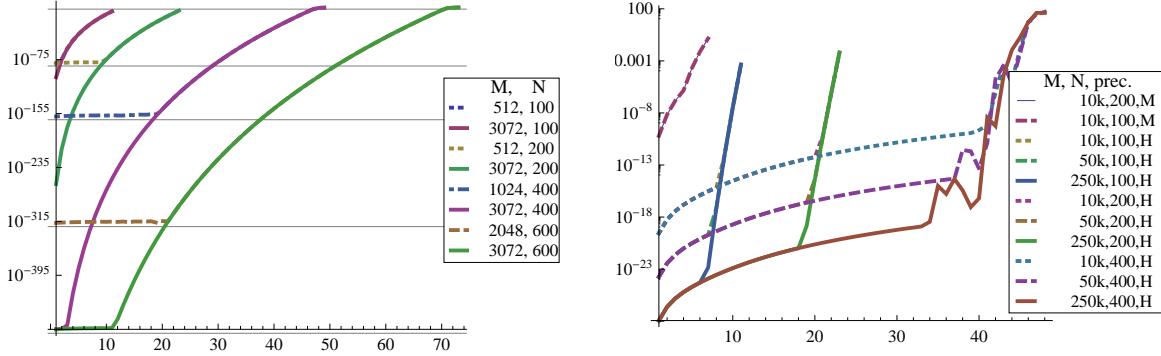


Figure 3: Absolute errors of the approximate eigenvalues in Example 4.4 obtained using different number of formal powers for approximating the exact characteristic equation (parameter N) and using Clenshaw-Curtis integration (on the left graph) and using the Newton-Cortes integration (on the right graph). M corresponds to the number of points used for representing the integrand, H means 64 digit precision and M means machine precision. The horizontal lines on the left graph show the errors of the particular solutions used for the calculation of the formal powers.

4.4 Spectral problems for pencils

In this subsection we consider several examples in which the right-hand side of equation (3.1) includes a derivative of the unknown function at the spectral parameter or depends polynomially on the spectral parameter.

The first two considered problems are from [2], [3] and belong to so-called second-order linear pencils.

Example 4.5. Consider the following problem [3, Example 3.3].

$$\begin{cases} -y'' + x^2 y = \lambda(2iy' + y), & 0 \leq x \leq 1, \\ y'(0) + i\lambda y(0) = 0, & y'(1) + i\lambda y(1) = 0. \end{cases} \quad (4.5)$$

The problem is self-adjoint and possesses a discrete real spectrum. With the help of Mathematica software we found the characteristic equation of the problem is given by the expression

$$(\lambda^2 + \lambda - 1) {}_1F_1\left(\frac{1}{4}(5 - \lambda(\lambda + 1)); \frac{3}{2}; 1\right) + {}_1F_1\left(\frac{1}{4}(1 - \lambda(\lambda + 1)); \frac{1}{2}; 1\right) = 0,$$

where ${}_1F_1$ is the Kummer confluent hypergeometric function.

We computed two particular solutions of (2.1) using the SPPS representation with $N = 100$ formal powers and $M = 10001$ points for the evaluation of the involved integrals by the Newton-Cortes 6 point formula, afterwards we used these particular solutions to compute $N = 100$ formal powers and to find the roots of the polynomial approximating the exact characteristic equation, spectral shift technique was used to obtain the higher index eigenvalues. The obtained eigenvalues together with the exact ones and the results from [2] and [3] are presented in Table 4. Note that our results are significantly better than the results from [2] and are comparable with the ones from [3]. However it should be mentioned that the approximations of the characteristic function of the problem (4.5) from [2] and [3] do not lead to an automatic approximation of the eigenfunctions; require some analytic precomputation as well as the solution of a large number of initial value problems which the authors of [2] and [3] performed by means of Mathematica with a required accuracy. Meanwhile the results delivered by the modified SPPS method were obtained using machine precision, did not require any analytic precomputation and include the eigenfunctions as well.

Example 4.6. Consider the following boundary value problem [3, Example 3.1].

$$\begin{cases} -y'' + q(x)y = \lambda(2iy' + y), & 0 \leq x \leq 1, \\ y(0) = 0, & y'(1) + i\lambda y(1) = 0, \end{cases} \quad (4.6)$$

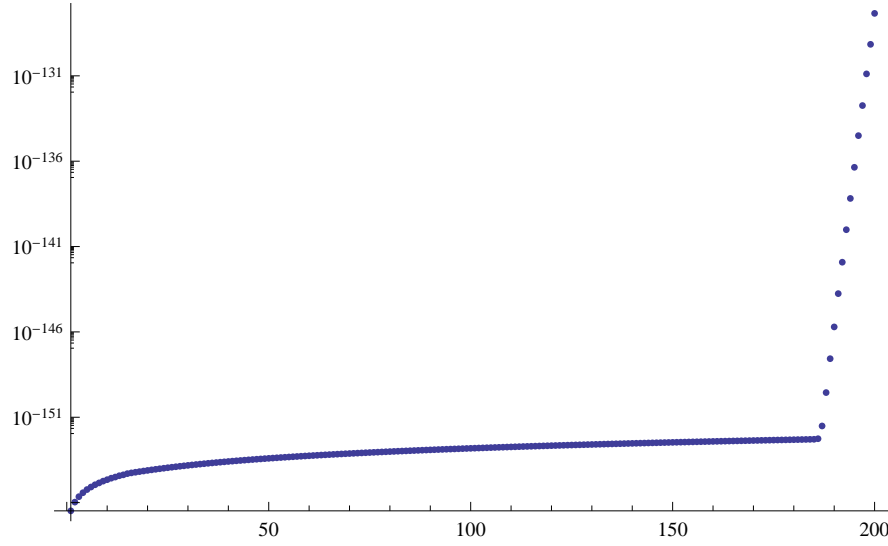


Figure 4: Absolute errors of the first 200 approximate eigenvalues in Example 4.4 obtained by the modified SPSS method applying the spectral shift technique.

n	λ_n (our method)	λ_n (exact)	λ_n ([2])	λ_n ([3])
-25	-75.90209254554286	-75.90209254550119		
-10	-28.78465916307922	-28.78465916308716		
-5	-13.08969157402720	-13.08969157402805		
-3	-6.830508103259227	-6.830508103259007		
-2	-3.741923372554198	-3.741923372554521	-3.7419233703827506	-3.7419233725545213
-1	-1.258249036460409	-1.2582490364604132	-1.2582490390569894	-1.2582490364604124
0	0.258249036460413	0.2582490364604132	0.2582490344106217	0.25824903646041525
1	2.741923372554577	2.741923372554521	2.741923371301097	2.7419233725545213
2	5.830508103259199	5.830508103259007	5.830508103873908	5.8305081032590085
3	8.955988815983204	8.955988815983707		
5	15.22658797653006	15.22658797653187		
10	30.92521763113015	30.92521763112857		
25	78.04353040058767	78.04353040632336		

Table 4: The eigenvalues of the problem (4.5) (Example 4.5).

where

$$q(x) = \begin{cases} 1, & 0 \leq x \leq 1/2, \\ 0, & 1/2 < x \leq 1. \end{cases}$$

This problem is not covered by Theorem 3.7, however it can be solved by the modified SPSS representation according to Remark 2.11. There seems to be some error in [2], [3] because the reported results are not the eigenvalues of the problem (4.6). With the help of Wolfram Mathematica we found that the characteristic equation of the problem (4.6) is given by the expression

$$\sqrt{\lambda^2 + \lambda} \tanh\left(\frac{1}{2}\sqrt{-\lambda(\lambda+1)}\right) \tanh\left(\frac{1}{2}\sqrt{1-\lambda(\lambda+1)}\right) + \sqrt{\lambda^2 + \lambda - 1} = 0. \quad (4.7)$$

We applied the modified SPSS method to this problem using the spectral shift technique computing both the particular solutions and the first 100 formal powers using $M = 10001$ for all involved integrals and performing integrations separately on each segment of continuity of the potential q . The calculated eigenvalues together with the exact ones obtained from (4.7) and with the resulted absolute errors are presented in Table 5.

n	λ_n (our method)	λ_n (exact)	Abs. error
-25	-77.4738498134661	-77.4738498206540	$7.8 \cdot 10^{-9}$
-10	-30.3579741391681	-30.3579741391157	$6.2 \cdot 10^{-11}$
-5	-14.6624304044055	-14.6624304044072	$1.9 \cdot 10^{-12}$
-3	-8.39761752583675	-8.39761752583497	$3.9 \cdot 10^{-12}$
-2	-5.30260260783015	-5.30260260783027	$2.5 \cdot 10^{-12}$
-1	-2.20110385479012	-2.20110385479002	$1.1 \cdot 10^{-13}$
0	1.20110385479006	1.20110385479002	$3.7 \cdot 10^{-14}$
1	4.30260260783056	4.30260260783027	$2.8 \cdot 10^{-13}$
2	7.39761752583498	7.39761752583497	$1.4 \cdot 10^{-12}$
3	10.5317097032223	10.5317097032191	$3.5 \cdot 10^{-12}$
5	16.8012911248982	16.8012911248964	$1.0 \cdot 10^{-11}$
10	32.4978603143171	32.4978603143055	$1.2 \cdot 10^{-11}$
25	76.4738498191705	76.4738498206540	$7.0 \cdot 10^{-9}$

Table 5: The eigenvalues of the problem (4.6) (Example 4.6).

For the next example we considered the following boundary value problem

$$\begin{cases} \frac{\partial}{\partial s} (A(s) \frac{\partial u}{\partial s}) - \frac{\partial^2 u}{\partial t^2} - p(s) \frac{\partial u}{\partial t} = 0, \\ u(0, t) = 0, \\ \frac{\partial u}{\partial s} \Big|_{s=l} + \nu \frac{\partial u}{\partial t} \Big|_{s=l} + \mu \frac{\partial^2 u}{\partial t^2} \Big|_{s=l} = 0, \end{cases}$$

describing small transverse vibrations of a string of stiffness $A(s)$ with a damping coefficient $p(s) > 0$. Here $u(s, t)$ is the transverse displacement and $l > 0$ is the length of the string. The left end of the string is fixed and the right end is equipped with a ring of mass $\mu > 0$ moving in the direction orthogonal to the equilibrium position of the string. The damping coefficient of the ring is $\nu > 0$. Similar problems were considered in various papers where theoretical results on direct and inverse problems were obtained, see, e.g., [12], [26], [27]. Substituting $u(s, t) = v(\lambda, s)e^{i\lambda t}$ we obtain the system for the amplitude function $v(\lambda, s)$.

$$\begin{cases} (A(s)v'(\lambda, s))' + \lambda^2 v(\lambda, s) - ip(s)\lambda v(\lambda, s) = 0, \\ v(\lambda, 0) = 0, \\ v'(\lambda, l) + i\nu\lambda v(\lambda, l) - \mu\lambda^2 v(\lambda, l) = 0. \end{cases} \quad (4.8)$$

The equation in (4.8) is of the type (3.1). In the case of a constant $p(s) \equiv p$ the problem can be reduced to a Sturm-Liouville problem by a change of the spectral parameter, however for a non-constant damping $p(s)$ the equation should be solved as a pencil.

Example 4.7. To be able to compare the approximate eigenvalues produced by the modified SPPS method with the exact ones we have chosen the following parameters: $A(s) \equiv 1$, $p(s) = s$, $\mu = \nu = 1$ and $l = 1$. For these parameters we were able to find with the help of Mathematica software the exact characteristic equation

$$\begin{aligned} \frac{\pi}{\sqrt[3]{i\lambda}} \left(\text{Bi}((i\lambda)^{4/3}) \left(\lambda(\lambda - i) \text{Ai}((i\lambda + 1)\sqrt[3]{i\lambda}) - \sqrt[3]{i\lambda} \text{Ai}'((i\lambda + 1)\sqrt[3]{i\lambda}) \right) + \right. \\ \left. \text{Ai}((i\lambda)^{4/3}) \left(\sqrt[3]{i\lambda} \text{Bi}'((i\lambda + 1)\sqrt[3]{i\lambda}) - \lambda(\lambda - i) \text{Bi}((i\lambda + 1)\sqrt[3]{i\lambda}) \right) \right) = 0, \end{aligned} \quad (4.9)$$

where $\text{Ai}(x)$ and $\text{Bi}(x)$ are the Airy functions. In Table 6 we present the approximate eigenvalues produced by the modified SPPS method with $N = 100$ and $M = 10001$ and with the use of the spectral shift technique, the exact eigenvalues obtained from the characteristic equation (4.9) with the help of Mathematica's function **FindRoot** and the absolute errors of the approximate eigenvalues compared to the exact ones. The eigenvalues are symmetric with respect to the imaginary axis, so we included only the eigenvalues with the positive real part. Note that our method allows one to obtain more eigenvalues, however Mathematica was unable to find more zeros of the characteristic equation.

n	λ_n (our method)	λ_n (exact)	Abs. error
1	$0.724600759561354 + 0.465512975730082i$	$0.724600759561355 + 0.465512975730082i$	$1.1 \cdot 10^{-15}$
2	$3.41348175703277 + 0.269073728680318i$	$3.41348175703277 + 0.26907372868032i$	$2.1 \cdot 10^{-15}$
3	$6.43085017426924 + 0.255763443512501i$	$6.43085017426926 + 0.255763443512497i$	$2.4 \cdot 10^{-14}$
4	$9.52497224975746 + 0.252665874553727i$	$9.5249722497575 + 0.252665874553731i$	$3.8 \cdot 10^{-14}$
5	$12.6419970813013 + 0.251521276777511i$	$12.6419970813014 + 0.251521276777512i$	$4.8 \cdot 10^{-14}$
7	$18.9002072286181 + 0.250683194824278i$	$18.9002072286181 + 0.250683194824283i$	$2.5 \cdot 10^{-14}$
10	$28.3081715202515 + 0.250305060446283i$	$28.3081715202511 + 0.250305060446279i$	$3.4 \cdot 10^{-13}$
15	$44.0040711901387 + 0.250126347925522i$	$44.0040711901389 + 0.250126347925464i$	$2.4 \cdot 10^{-13}$
20	$59.7063095058408 + 0.250068647436092i$	$59.7063095058413 + 0.250068647435942i$	$5.8 \cdot 10^{-13}$

Table 6: The eigenvalues of the problem (4.8) (Example 4.7).

4.5 Spectral problems for Zakharov-Shabat systems

Zakharov-Shabat systems arise in the application of the inverse scattering transform method to non-linear Schrödinger equations, see, e.g., [1, 29, 30]. In this subsection we follow definitions and results from the recent papers [22, 21]. We consider a generalized Zakharov-Shabat system

$$\begin{cases} v_1' = \lambda v_1 + P v_2, \\ v_2' = -\lambda v_2 - Q v_1, \end{cases} \quad (4.10)$$

where v_1 and v_2 are unknown complex valued functions, $\lambda \in \mathbb{C}$ is a spectral parameter, Q and P are complex valued functions such that Q does not vanish, P is continuous and Q is continuously differentiable on the domain of interest. Substituting $v_1 = -\frac{1}{Q}(v_2' + \lambda v_2)$ into the first equation in (4.10) we obtain an equation of the form

$$\left(\frac{1}{Q}v_2'\right)' + P v_2 = \lambda \frac{Q'}{Q^2} v_2 + \lambda^2 \frac{1}{Q} v_2. \quad (4.11)$$

Equation (4.11) is of the form (3.1), hence we can apply the results of Section 3 to obtain the solution of the Zakharov-Shabat system.

Recall that the eigenvalue problem for the system (4.10) consists in finding such values of the spectral parameter λ for which there exists a non-trivial Jost solution. In particular, when the potentials Q and P are compactly supported and non-vanishing on $[-a, a]$ (a situation which usually arises when truncating the infinitely supported and rapidly decreasing potentials) the eigenvalue problem reduces to finding such values of λ (with $\operatorname{Re} \lambda > 0$) for which there exists a solution of (4.10) on $(-a, a)$ satisfying the following boundary conditions (see, e.g., [22])

$$v_1(-a) = 1, \quad v_2(-a) = 0, \quad (4.12)$$

$$v_1(a) = 0. \quad (4.13)$$

Let f and g be two particular solutions of (4.11) for some $\lambda = \lambda_0$ satisfying the conditions of Theorem 3.7 and the solutions u_1 and u_2 be constructed by (3.35) using $x_0 = -a$ as the initial point in Definition 3.2. Then the general solution of (4.11) has the form $v_2 = c_1 u_1 + c_2 u_2$ and it follows from (4.12) and (3.30) that $c_1 = 0$, while from the boundary condition for the function $v_1 = -\frac{1}{Q}(v_2' + \lambda v_2)$ we obtain that $c_2 = -1$. Hence due to (4.13) the characteristic equation of the spectral problem reduces to

$$0 = v_1(a) = -\frac{1}{Q(a)}(v_2'(a) + \lambda v_2(a)) = \frac{1}{Q(a)}(u_2'(a) + \lambda u_2(a)).$$

Multiplying both sides by $Q(a)$ we obtain that the eigenvalues of the spectral problem coincide with zeros of the characteristic function

$$\begin{aligned} \Phi(\lambda) &= \rho \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n (g'(a) F_{2n}(a) - f'(a) G_{2n}(a)) + \lambda \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n F_{2n+1}(a) \\ &= \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n \left(\rho (g'(a) F_{2n}(a) - f'(a) G_{2n}(a)) + F_{2n-1}(a) + \lambda_0 F_{2n+1}(a) \right). \end{aligned} \quad (4.14)$$

Example 4.8. Consider the following problem [6]

$$\begin{cases} i\varepsilon v' = qw + \lambda v, \\ i\varepsilon w' = \bar{q}v - \lambda w, \end{cases} \quad (4.15)$$

where the potential q is given by

$$q(x) = A(x)e^{iS(x)/\varepsilon}, \quad A(x) = S(x) = \operatorname{sech}(2x),$$

\bar{q} denotes the complex conjugate of q and ε is a small parameter. According to [6] the problem possesses a finite set of eigenvalues having a “Y”-shape in the complex domain.

After division by $i\varepsilon$, (4.15) reduces to the Zakharov-Shabat system (4.10) with the spectral parameter $\tilde{\lambda} = \lambda/i\varepsilon$. This problem was numerically solved in [21, Example 4.10] using machine-precision arithmetic by means of the original SPPS representation for several values of $\varepsilon \geq 0.063$. In [6] the graphs of the eigenvalues on the complex plane are presented for values of ε as small as 0.023. Such small values of ε presented difficulties in [21, Example 4.10]. It was not possible to compute sufficiently many formal powers to obtain all the eigenvalues without using the spectral shift technique, the larger index formal powers became smaller than the smallest numbers in double precision. The spectral shift technique did not help either because of the rapid growth followed by the rapid decay of the particular solutions used for spectral shifts, similar difficulty as in the Coffey-Evans example [20, Example 7.5]. One possibility to overcome these difficulties in the framework of the original SPPS method consists in using arbitrary precision arithmetic. However even in this case the Clenshaw-Curtis integration formula allowed us to calculate only a few formal powers accurately, meanwhile the use of the Newton-Cotes integration formula led to elevated computational times.

The modified SPPS representation allowed us to overcome the main computation difficulty of the original SPPS representation — nearly vanishing solutions. We truncated the potential to the segment $[-8, 8]$ and computed two particular solutions of equation (4.11) along with more than 2000 formal powers using the Clenshaw-Curtis integration formula. Such amount of formal powers is sufficient to obtain all eigenvalues of the problem (4.15) for all values of ε reported in [6] directly from the truncated characteristic function (4.14). We confirmed the smaller eigenvalues using the spectral shift method. For the larger eigenvalues the spectral shift method failed to produce reliable results with the parameters used because the particular solutions reveal a computationally difficult behavior, starting at 1 they grow to more than 10^{40} and then decay. All calculations were performed in Mathematica 8 using arbitrary precision arithmetic. On Figure 5 we present the graphs of the obtained eigenvalues for $\varepsilon = 0.025$ and $\varepsilon = 0.0223$, smallest values from [6], and in Table 7 we present the approximate eigenvalues for $\varepsilon = 0.025$.

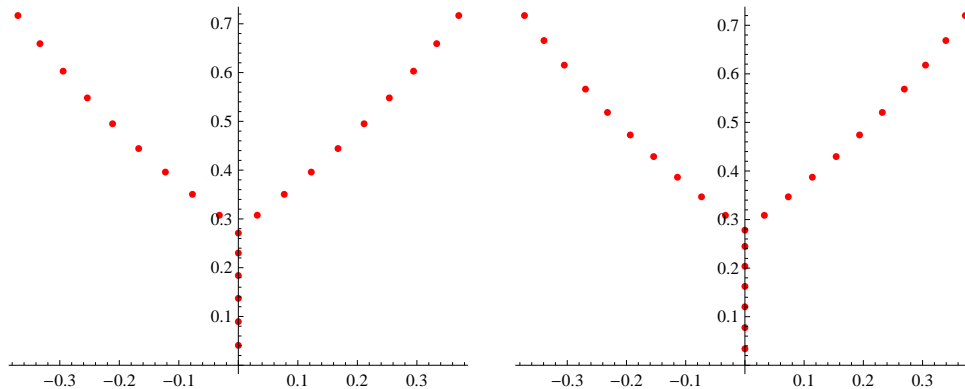


Figure 5: Graphs of the eigenvalues of the problem (4.15) from Example 4.8 for $\varepsilon = 0.025$ (on the left) and for $\varepsilon = 0.0223$ (on the right).

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n	λ_n (our method)
1	0.0407631404708347818 <i>i</i>
2	0.0894375732679124748 <i>i</i>
3	0.1371637819552007166 <i>i</i>
4	0.183974867838984848 <i>i</i>
5	0.230058316868567325 <i>i</i>
6	0.270992331790330981 <i>i</i>
7, 8	$\pm 0.031821868157610443 + 0.307581835672991608i$
9, 10	$\pm 0.077099873305919148 + 0.350414351766500910i$
11, 12	$\pm 0.122549274277416703 + 0.396004265795121343i$
13, 14	$\pm 0.167461129865269703 + 0.444273217295649703i$
15, 16	$\pm 0.211303802258405430 + 0.495044232076272957i$
17, 18	$\pm 0.253691811351361979 + 0.548028112642247410i$
19, 20	$\pm 0.294386770221071665 + 0.602887000706132156i$
21, 22	$\pm 0.333275636341542323 + 0.659282807236860406i$
23, 24	$\pm 0.370339678528560140 + 0.716906655582204397i$

Table 7: The eigenvalues of the problem (4.15) for $\varepsilon = 0.025$ (Example 4.8).

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